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(54) Title: A METHOD FOR PERFORMING RESTRAINED DYNAMICS DOCKING OF ONE OR MULTIPLE SUBSTRATES ON MULTI-SPECIFIC ENZYMES

(57) Abstract: The present invention relates to a method for performing restrained dynamics docking of one or several substrates having allosteric or synergistic effect on enzymes presenting multipspecific and flexible active site. It also concerns a method for determining the 3D-substrates, which is the case for multispecific enzymes such as cytochrome P450, and specifically to cytochrome P450 3A4 and P450 3A7.





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A method for performing restrained dynamics docking of one or multiple substrates on multi-specific enzymes

The present invention relates to a method for performing restrained dynamics docking of one or several substrates having allosteric or synergistic effect on enzymes presenting multispecific and flexible active site. It also concerns a method for determining the 3D-structure of active sites that are flexible and can adapt to different substrates, which is the case for multispecific enzymes such as cytochrome P450.

As of today, various computer graphics systems allow to generate molecular models of large molecules such as proteins from the PDB structural data obtained using X-ray crystallography and NMR. We can cite for example MODELLER, COMPOSER, MATCHMAKER (Tripos), or 3D graphical environments for molecular modeling such as SYBYL (Tripos) or INSIGHT II (Accelrys).

Substrates as well as inhibitors or agonists often act by binding to particular regions of an enzyme or receptor referred as the active site. In industry, the purpose of using these 3D models is to assess the main features of the molecules which are involved in the binding to the active site. New molecules that fit the active site can be designed.

Biological interactions are not possible without flexibility and motion. One of the principal tools in the theoretical study of motion in biological molecules is the method of molecular dynamics simulations (MD). This computational method calculates the time dependent behavior of a molecular system (Karplus and McCammon, 2002). MD simulations have provided detailed information on the fluctuations and conformational changes of proteins and nucleic acids. These methods are now routinely used to investigate the structure, dynamics and thermodynamics of biological molecules and their complexes. They are also used in the determination of structures from x-ray crystallography and from NMR experiments. The molecular dynamics simulations can be used to recreate the successive events in the binding process of a molecule, and thermodynamic parameters implicated in such process can therefore be derived, which is of great interest in the design of active molecules.

Nevertheless, the methods proposed in the art are based on a relatively low level of calculations of few parameters. It relies only on the molecule energy constrained with a fixed geometry. It relies only on the interaction energy between the molecule and the active site frozen in a fixed geometry.

5 Consequently, there is a need for a model replicating *in silico* the natural process of molecular interactions.

The method according to the invention provides both minimizations and molecular dynamics calculations. More specifically, it provides a new approach which is more appropriate to flexible structures, hereafter referred as "restrained dynamics docking" or "soft-restrained restrained dynamics docking". This technique employs constrained dynamics simulations, where the only constraints are active sitesubstrate distances.

For example, to explain and predict drug metabolism in organisms, in which the cytochrome P450 (CYP) superfamily of haem-thiolate enzymes plays a central role, it is of large interest to dispose of a molecular picture of the binding sites responsible for the biotransformation. Efficiency of the prediction is then directly related to the molecular precision of the model, which resolution must be obtained at the atomic level to exploit the model for further docking studies.

In mammalian, hepatic cytochrome P450s constitute the major enzymes involved in the metabolism of exogenic compounds. Among them, isozymes of the CYP3 family (such as CYP3A1 and 3A2 in rat, and CYP3A4, CYP3A5, CYP3A7, CYP 3A43 in human) are known to metabolize the majority of drugs in clinical use. These are multi-specific enzymes, able to metabolize a large variety of structurally diverse chemicals or substrates including steroids, linear or cyclized peptides (Delaforge et al. 1997, Delaforge et al. 2001, Aninat et al. 2001), generally fairly lipophilic, within a broad range of molecular sizes from testosterone (Mw 288) to cyclosporin A (Mw 1203).

The inventory of known substrates for CYP 3A contains a large variety of different molecules having apparently no common structural factors. Actually it can be estimated that more than five hundred utilized drugs can be recognized and metabolized by CYP 3A (Guengerich 1995, Wrighton et al. 2000, Lewis 2001). Closer inspection of the precise transformations catalyzed by CYP 3A indicates that there is an important regio- and stereo-selectivity for each substrate. The active site

can accommodate relatively rigid substrates such as aflatoxin derivatives or steroids, that are oxidized almost exclusively at a precise position. Thus CYP 3A4 catalyzes the testosterone oxidation exclusively at the 6β position, whereas CYP 3A7 oxidizes dehydroepiandrosterone (DHEA) or its 3 sulfate conjugate exclusively on the 16α position (see Figures 4A and 4B). In addition to such small substrates, CYP 3A metabolize also large molecules such as cyclosporin A (MW 1202), macrolide antibiotics (MW around 600) or ergot derivatives (MW from 500 to 700).

The recognized substrates can have endogenous origin such as steroids or can be drugs or compounds found in food. For example, grapefruit juice contains bergamottin derivatives having specific CYP 3A inhibitory activities (Schmiedlin-Ren et al. 1997). Linear peptides (Delaforge et al. 2001, Hosea et al. 2000) or cyclized peptides (Delaforge et al. 1997) containing from 2 aminoacids (called diketopiperazine, Delaforge et al. 2001, Aninat et al. 2001) to 11 amino-acids (e.g. cyclosporin) are also recognized.

Following this wide range substrate recognition, a tentative subclassification was established leading to a multi-site hypothesis (Hosea et al. 2000, Ekins et al. 2003) consisting of at least 2 or 3 binding zones in the active site. This hypothesis has been established on the facts that CYP 3A shows often atypical hyperbolic kinetic constants and is thus unable to reach saturation. In addition, the presence in the active site of a second substrate having a different molecular nature lead to either no modification or increased metabolism of both substrates. Such allosteric effects have been clearly described in the case of simultaneous metabolism of steroids such as testosterone and α -natphtoflavone.

Consequently, any molecular model describing correctly the multiple substrate specificity (that takes into account large variations in molecular size and chemical structures), and substrate cooperativity effects within the active site (when two or more drugs interact), is of considerable scientific and industrial interest. Such a molecular model must be able to rationalize the binding of the diverse known substrates, and the orientations of the molecules in the binding site that account for their known positions of metabolism (such as N-demethylations, benzylic hydroxylations etc.).

CYP3A4 is considered as the main hepatic form and is found in a wide variety of human organs such as intestine, brain or skin. CYP 3A5 is also present in liver and is the major 3A form present in the kidney. The 3A5 isoform is subject to genetic polymorphism. CYP 3A7 is the major 3A isoform present in the foetus whereas CYP3A43 is mainly located in adult prostate or testis. These isoforms share amino acid identities higher than 70%. (Westlind-Johnsson et al. 2003, Gellner et al. 2001, Koch et al. 2002). It is currently accepted that CYP3A4 is the most active isoform for classical P450 3A substrates whereas recent data (Williams et al. 2002) demonstrate equal or slightly reduced activity for CYP3A5 and a significantly lower metabolism capability for CYP3A7 as compared to CYP3A4. Additionally, differences have been observed in term of oxidative regioselectivity of the CYP3A7 compared to other isoforms. As an example, CYP3A7 metabolizes intensively DHEA and especially its sulfate conjugate derivative whereas CYP3A4 is a poor metabolizer. The oxidation by CYP3A7 occurs mostly in the 16a position of DHEA. In contrast, CYP3A7 metabolizes testosterone in both 6β and 16α position whereas CYP3A4 or 3A5 metabolize it almost exclusively in the 6B position (Inoue et al. 2000).

At the contrary of the P450 3A subfamily, other P450 isoforms have more rigid active site, as suggested by the narrow range of recognized substrates or inhibitors. These P450 isoforms recognize generally a small number of substrates or inhibitors having in common the same shape (i.e. P450 1A isoforms), or the same charge (i.e. CYP 2B, 2C or 2D isoforms), or the same chemical nature such as steroids (i.e. CYP19 or CYP21 isoforms) or lipids (i.e. CYP 4 family).

As no high-resolution 3D structure of CYP3A is today publicly available, due to continuing difficulties in promoting crystallization of intrinsic membrane proteins or due to an unusual conformational flexibility that would explain how CYP3A can accommodate various substrates, it is necessary to rebuild a 3D model structure, integrating the known biochemical data of CYP3A and the structural data of other members of the CYP superfamily. X-ray crystallographic determinations of several bacterial P450 enzymes in the 1990s (see Table 1 for a summary of structural data) have stimulated numerous attempts in modeling microsomal P450S such as human CYP3A4. The chapter 6 of the book "Guide to Cytochromes P450: structure and function" written by David F.V. Lewis reviews the current status of structural and

modeling investigations of the P450 family (Lewis 2001). This review was however written just before the release of the first mammalian P450 structure (2C5), still today the only one mammalian template available.

Table 1

CYP isoform crystallized	PDB code (resol.)	Organism	Function	No of residues	Reference
P450 cam (complexed by CO+camphor)	3cpp (1.9 Å)	Pseudomonas Putida	Camphor Monooxygenase	414	(Poulos et al. 1985) (Raag and Poulos 1989)
P450 terp	1cpt (2.3 Å)	Pseudomonas sp.	Alpha-terpineol hydroxylation	412	(Hasemann et al. 1994)
P450 BM3	2hpd (2 Å)	Bacillus megaterium	Fatty acid monooxygenase	471	(Ravichandran et al. 1993)
P450 cryF (6-deoxyerythro -nolide B bound)	loxa (2.1 Å)	Saccharopolyspora erythraea	Erythromycin biosynthesis 6S- hydroxylation of 6- deoxyerythronolide B	403	(Cupp-Vickery and Poulos 1995)
P450 nor	lrom (2 Å)	Fusarium oxysporum (denitrifying fungus)	Nitric Oxide Reductase	403	(Park et al. 1997)
P450 2C5	1dt6 (3 Å)	(membrane-type Mammalian) Rabbit	Progesterone 21- Hydroxylase	473 (487)	(Williams et al. 2000)
P450 CYP119 4-Phenylimidazole Bound	1f4t (1.93 Å)	Sulfobolus Solfactaricus Thermophilic bact.	unknown	368	(Yano et al. 2000)
P450 CYP51	1e9x (2.1 Å)	Mycobacterium - Tuberculosis	14 α-sterol demethylase	455 (451)	(Podust et al. 2001)
4-Phenylimidazole Bound					

Table 1: the eight X-ray crystal structures of P450s available in 2002: six bacterial, one fungal (P450 nor), one mammalian (CYP2C5). The P450_{cam}, P450_{terp}, P450_{eryF}, P450_{nor} belong to class I P450s enzymes, whereas P450_{BM3} belongs to class II enzymes, like microsomal enzymes CYP2C5 and 3A. P450_{BM3} structure is therefore a priori more relevant to rebuilding a structural model of CYP3A, but since the CYP2C5 X-Ray structure has been released, it became obvious that the structural homology between the other bacterial enzymes and microsomal enzymes was better than expected from the poor homology of primary structure (< 25% identity). Then, the relevance of using class I and class II structures together for rebuilding models of class II P450s was no more questionable. In the two examples described in the present invention, the structural model of human CYP3A4 was rebuilt using the six

first structures listed above, with no preference in the structural alignment, and the structural model of human CYP3A7 was rebuilt using four structures among those listed above with again no preference in the structural alignment, *i.e.* P450_{BM3}, P450 EryF, P450 2C5 and CYP51, one of the last published structural sets. CYP119 was not incorporated into the modeling process.

All the proposed models of CYP3A4 obtained by homology modeling are thus so far based on bacterial crystal structure templates: the first was proposed by Ferenczy and Morris and used the X-ray structure of bacterial P450_{cam} as unique template structure (Ferenczy and Morris 1989). Another model was built later by David F.V. Lewis, using also a unique template structure, the P450_{BM3} structure, which was supposed to be more relevant as a template since this P450 was the only one class II enzyme with known three-dimensional structure (Lewis et al. 1996). A third model, based on a multiple structure template, was built by Szklarz and Halpert, using the four first X-ray crystal structures available P450cam, P450terp, P450_{ervF}, and P450_{BM3}. This four-bacterial template approach strategy is closer to our rebuilding strategy, but was still missing some relevance in the absence of a mammalian template. In our hands, the incorporation of the mammalian 2C5 crystal structure into rebuilding steps of models of cytochrome P450 3A proved to be decisive. Inclusion of 2C5 crystal structure had indeed a profound effect on the structural alignment with the five non-mammalian structures, resulting in a different topology of the active site and a marked divergence between the model and each individual template. The advantage of our multiple-template approach resides essentially in the availability of a final template that can be used to rebuild various mammalian cytochromes P450. Up to now there is no available crystal structure or structural model of human CYP3A5, CYP 3A7, CYP3A43 or other mammalian CYP3A.

More recently, two new bacterial P450 crystal structures emerged in the literature (Table 1): CYP51 (PDB code 1e9x), from *Mycobacterium tuberculosis*, that catalyzes the oxidative removal of 14α-methyl group from sterol precursors in sterol biosynthesis in yeast and fungi (ergosterol), plants (phytosterol) and mammals (cholesterol), for its potential in the design of antifungal agents (Podust et al. 2001). And CYP119 (PDB code 1f4t), from the thermophilic archaeon *Sulfolobus solfataricus*, the first P450 identified in *Archaea*, for its interest in

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understanding the enhanced thermal stability of the structure, especially in the region of the active site (Yano et al. 2000). Those two structures have been shown to exhibit the typical bacterial P450 fold, with some exceptions in the topology. They have not been included as structural templates in the modeling steps of the CYP3A4 model described in example 1. The names of newly discovered P450s follow the now accepted nomenclature of David R. Nelson (Nelson 1999).

The protein databank (Brookhaven Protein Databank, http://www.rcsb.org/pdb/) currently indicates that there are 76 separate crystal structures available for the eight crystallized P450s, plus 7 crystal structures on hold (Sept 1st, 2002), the majority of which containing either bound substrates or inhibitors. Table 1 provides the relevant information about the structural templates used for human CYP3A model rebuilding. The idea behind homology modeling is that proteins belonging to the same functional class and showing a strong sequence identity, adopt a similar fold (review in (Hilbert et al. 1993)). Known analogous structures are then used to 15 generate a template or parent structure for the unknown protein to be modeled. The reliability of the various methods employed depend mostly on the number of experimental 3D structures that can be aligned. Knowing that for pairs of distantly related proteins (with residue identity of about 20%) the regions having the same fold will represent less than half of each molecule, the regions where the folds differ will predominate, and the divergence of sequence must be compensated by a higher number of homologous proteins to align (Chothia and Lesk 1986). Below 50% of sequence identity, the deviation in structurally not conserved regions becomes significant, and loop regions are difficult to predict. It is generally accepted that below 20% of sequence identity, the prediction turns out to be hazardous, and fold assignment methods are best replaced by ab initio methods, that ideally attempt to predict the native structure only from the primary sequence of the protein to be modeled. But produced models so far had the correct fold for only a few small protein domains (Sanchez et al. 2000).

The strategy of model rebuilding in the P450 family is strongly driven by the low degree of homology between bacterial and mammal cytochrome P450s (Table 2).

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Fable 2

ايم	FUSOX										
NON A	<u> </u>										
CPXJ	SACER										32.7 % 395 aa
CPXB_	BACME									22.6 % 389 aa	31.5 % 23.0 % 409 aa 265 aa
CPXL_	PSESP								24.0 % 363 aa	28.6 % 420 aa	31.5 % 409 aa
-cPXA-	PSEPU							27.4 % 398 aa	23.1 % 485 aa	24.0 % 391 aa	29.0 % 379 aa
	RABIT						23.3 % 21.3 % 21.9 % 26.6 % 24.2 % 335 aa 399 aa 407 aa 387 aa 480 aa	27.8 % 29.3 % 24.4 % 446 aa 409 aa 451 aa	24.5 % 22.7 % 396 aa 480 aa	25.5 % 26.0 % 27.7 % 30.8 % 24.4 % 24.0 % 28.6 % 22.6 % 415 aa 334 aa 423 aa 396 aa 443 aa 391 aa 420 aa 389 aa	23.7% 22.9% 23.1% 27.7% 21.4% 29.0% 31.5% 354 aa 415 aa 442 aa 379 aa 351 aa 379 aa 409 aa
epxwepxes	SULSO					23.5 % 344 aa	26.6 % 387 aa	29.3 % 409 aa	24.5 % 396 aa	30.8 % 396 aa	27.7 % 379 aa
TISdo	MYCTU				25.7 % 385 aa	23.4 % 427 aa	21.9 % 407 aa	27.8 % 446 aa	27.1 % 443 aa	27.7 % 423 aa	22.9 %, 23.1 % 415 aa 442 aa
CP34_	HUMAN	認。過		26.9 % 405 aa	24.5 % 25.4 % 25.7 % 330 aa 410 aa 385 aa	27.9 % 28.4 % 481 aa 497 aa	21.3 % 399 aa	24.8 % 24.4 % 452 aa 356 aa	29.9 % 445 aa	26.0 % 334 aa	22.9 %. 415 aa
CP37_	HUMAN		88 4 % 50 aa	27.7 % 26.9 % 372 aa 405 aa	24.5 % 330 aa	27.9 % 481 aa	23.3 % 335 aa	24.8 % 452 aa	31.8 % 409 aa	25.5 % 415 aa	23.7 % 354 aa
Swiss-Prot	entry name	CP37_HUMAN	CP34_HUMAN	CP51_MYCTU (CYP51)	CPXW_SULSO (CYP119)	CPCS_RABIT (CYP2C5)	CPXA_PSEPU (P450 cam)	CPXL_PSESP (P450 terp)	CPXB_BACME (P450 BM3)	CPXJ_SACER (P450 eryF)	NOR_FUSOX (P450 nor)
POB	epoo	n.s.	n.s.	1E9X	1F4T	1DT6	3CPP	ICPT	2HPD-A	10XA	IROM

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Table 2: Sequence identities between the various crystallized cytochrome P450s and human CYP3A4 and CYP3A7 using BLOSUM 62 matrix (source LALIGN, http://www.infobiogen.fr/services/analyseq/cgi-bin/lfastap_in.pl, algorithm of Huang and Miller LALIGN that finds the best local alignments between two sequences, version 2.1u03 April 2000, published in *Adv. Appl. Math.* 1991, 12: 373-381). The P450 BM3 structure, Swissprot code name CPXB_BACME, corresponds to the structure of a fusion protein of P450 and a reductase domain, so that it displays twice the number of residues.

- Our global scheme, which steps are described hereafter, is founded on a combination of methods developed in the literature for different purposes in protein structure determination studies. The principle of the primary steps, until the generation of a correct alignment of P450 primary sequences, is described in Jean et al. 1997. The last steps are summarized in Loiseau 2002.
- Therefore, in a first object, the invention relates to a method for designing a 3-dimentional (3-D) model of a protein, the 3-D representation of at least three family members has already been experimentally obtained, [said 3-D representation presenting similarities], comprising the steps of:
- a. identification of common structural blocks (CSBs) among said members of said family,
 - b. alignment of the amino-acids primary sequence of said family members according to said structural similarities, represented by said CSBs, in order to obtain a first alignment,
- c. alignment of said protein as compared on said first alignment, in order to obtain a second alignment, wherein:
 - i. alignment of said protein is performed in order to optimize the amino-acids alignment between said protein and said first alignment, when one or more consensus amino-acid exists in said aligned CSBs in said first alignment, and in the amino-acid sequence of said protein, said consensus amino-acids are anchors of said second alignment,
 - ii. no insertion or deletion of amino-acids can be performed in the aligned CSBs, wherein insertion or deletions are possible in out-of-block regions, if better to align the primary amino-acids sequences,

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- d. definition of the 3-D structure of CSBs of said protein, according to the 3-D structure of the CSBs of said family members,
- e. definition of the global constraints (distance and angular constraints) derived from the comparisons of the structural templates in CSBs, and definition of the local constraints (distance and angular constraints) for the atoms of residues that are not structurally determined after step d. (that are not in the CSBs),
- f. selection of rotamers,
- g. determination of a family of 3-D model structures of said protein, taking into account said 3-D structure of CSBs obtained in step d., said global and local constraints defined in step e., and said rotamers defined in step f.,
- h. optimization of said family of 3-D models obtained in step g., by
- i discarding structures that present topological defects, and
- ii recalculating 3-D structures by taking electrostatic forces into account, and performing the method again from step c. downward, with modifications in the alignment between the primary sequence of said protein and said first alignment, when the obtained model structures do not satisfactorily account for known mutations having biological effects.
- In the present invention, the term "backbone atoms" refers to the C, N, C α , and O atoms of a protein that are common to all amino acid building blocks or involved in the peptide linkage. When the protein structure is described as a trajectory in internal coordinates such as α , τ angles, or is a low-resolution crystallographic structure, backbone atoms stand only for C α atoms of each residue.
- In the present invention, the term "similarities" is used in the search for structural fragments conserved between the template proteins, that is fragments that have similar local trajectories in the backbone internal coordinate space. Two protein fragments have "similar" local trajectories when they are matched according to two adjustable parameters, the mesh and the margin (Jean et al. 1997).
- In the present invention, the term "common structural blocks (CSB)" define the protein fragments of equal length that are found similar between all the template proteins in the internal coordinate representation.
- In the present invention, the term "first alignment" refers to the alignment imposed by the CSBs, that is the structural alignment between template proteins defined by

CSBs sequences. This alignment is totally independent on the primary sequence of the template proteins.

In the present invention, the term "out-of-block regions" designates all other protein fragments located out of and between the CSBs, *i.e.* that are not structurally conserved in the internal coordinate space. There is no information of sequence alignment for these regions (see in Figure 1 regions that are not colored), since they are not relevant for structural conservation. Out-of-block regions are passively reconstructed with the rest of the structure during the calculation steps.

In the present invention, the term "global constraints" refers to geometric constraints that are assigned to atoms of residues from CSBs, and that can be derived by computing all distance or angle information available within CSBs or between CSB.

In the present invention, the term "local constraints" refers to loose structural constraints that are assigned to residues of out-of-block regions, in order to restrict their backbone conformation to allowed regions of the Ramachandran diagram.

In the present invention, the term "rotamers" defines the low energy side-chain conformations of residues. The use of a library of rotamers allows determining or modeling a structure with the most likely side-chain conformations, saving time and producing a structure that is more likely to be correct.

20 For identification of CSBs between all selected 3D structures:

CSBs define the common local folds found similar in the template proteins, and are used as building blocks to set up the fold of the model (results in Loiseau 2002). The non conserved regions, that can be parts of secondary structures or non-structured regions as loops, will be rebuilt with no initial structural information.

For multiple alignment of crystalline P450s, on the basis of CSBs determination:

Once the structurally conserved elements are identified, a first structural alignment between the template proteins is derived. The following step involves the localization of these elements in the target sequence. Sequence pairwise comparisons between selected crystal structures and CYP3A (Table 2) show low sequence identity, so that online tools of multiple alignment such as CLUSTALW or PHD (Heidelberg) fail to produce an clear-cut alignment. Instead, local alignment tools, such as that described in Jean et al. 1997, were used to match the CSB profile to the target sequence, where a matrix is slid along the sequence and a

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score of similarity (based on a standard matrix such as BLOSUM62) is calculated for each position. Online tools of multiple alignment such as CLUSTALW 1.8 can be further used for assessment of accuracy.

The target sequence of human cytochrome P450 3A is thus aligned against the multiple alignment obtained from the CSBs. This produces the key sequence alignment which allows the generation of the template structure used for the rebuilding of the various CYP3A models. Following steps involve:

- 1) Generation of distance and dihedral angles constraints.
- 2) Selection of rotamers for side chains in CSBs.
- 3) Calculation of a set of structures using DYANA software. Loops are rebuilt between CSBs.
 - 4) Structure optimization under XPLOR software (Brünger 1992).

In a preferred embodiment, said 3-D representation of family members has been obtained by crystallography or NMR.

The alignment of said common structural blocks in steps **b**. and **c**. can be performed by use of the GOK software as described in Jean et al., 1997.

In addition, step d. is preferably performed according to the following rules:

- i. at a given position, when residues are identical between all the template structures and the target sequence, the 3D coordinates of the reference residues are purely assigned to the target residue,
- ii. When residues differ, only the coordinates of the backbone atoms are assigned $(C\alpha)$, and sometimes $C\beta$ or $C\gamma$ when they exist.

The definition of rebuilding global constraints in step e. is performed by using all available geometrical information intra- and inter-CSB (distances and angles), issued from the comparisons of the structural templates, each geometric constraint being defined as an interval. On another hand, the definition of local constraints for out-of-blocks residues is performed by analysis of the allowed regions in Ramachandran diagram.

Furthermore, distances and angles defining global constraints are preferably selected in step e. by the following rules:

- i. all distances for which the lower boundary is less than 8 Å,
- ii. all the distances involving at least one side-chain atom, to preserve the spatial arrangement between CSBs

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iii.all the distances involving atoms of any active group such as an heme group, to fix as much as possible the neighborhood of said active group, such as an iron atom.

The distance of 8 Å is chosen in order to reduce drastically the total number of constraints to take into account in the computation, and to allow to excessively constrain the model.

Angular constraints are preferably selected in step e. by the following rule:

i. dihedral angles ϕ and ψ of all residues located in CSBs are defined as constraints, given by the average values of corresponding ϕ , ψ angles in said family members +/- the calculated standard deviation.

To practice the method of the invention, rotamers in step f. can be selected from the couples according to the tables of Dunbrack and Karplus and step g. can be performed with the DYANA software, as described in Güntert et al, 1997.

In addition, the optimization in step h. comprises the use of the X-Plor software, as described in A. T. Brünger, X-PLOR, version 3.1.

The method according to the invention is particularly applicable to a cytochrome P450 subfamily 3A comprising mammal and human cytochromes P450 3A]

In a preferred embodiment, said mammal cytochrome P450 3A is selected from the group comprising CYP3A6 (SEQ ID N°14), CYP3A12 (SEQ ID N°16), CYP3A29

0 (SEQ ID N°17) and CYP3A13 (SEQ ID N°18).

In another preferred embodiment, said human cytochrome P450 subfamily 3A is selected from the group comprising CYP3A4 (SEQ ID N°11), CYP3A7 (SEQ ID N°15), CYP3A5 (SEQ ID N°12) and CYP3A43 (SEQ ID N°13).

The method is applicable as well to human cytochrome of the subfamily P450 3A4, wherein said family members that are used for performing said first alignment for designing a 3-D model of CYP3A4 are chosen from Nor (SEQ ID N° 1), Ery F (SEQ ID N° 2), terp (SEQ ID N° 3), Cam (SEQ ID N° 4), BM3 (SEQ ID N° 5) and 2C5 (SEQ ID N° 6).

The method is applicable as well to human cytochrome of the subfamily 3A7, wherein family members that are used for performing said first alignment for designing a 3-D model of CYP3A7 are chosen from Ery F (SEQ ID N° 2), BM3 (SEQ ID N° 5), CYP51 (SEQ ID N° 8) and 2C5 (SEQ ID N° 6).

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The method is applicable as well to other mammalian cytochrome P450 3A isoforms.

In a second object, the invention is directed to 3-D structure model of a protein, obtained by the method as described above.

- In a preferred embodiment, the protein is a cytochrome P450 subfamily 3A comprising mammal and human cytochromes P450 3A

 In another preferred embodiment, the protein is selected from the group comprising CYP3A6 (SEQ ID N°14), CYP3A12 (SEQ ID N°16), CYP3A29 (SEQ ID N°17) and CYP3A13 (SEQ ID N°18).
- In still another preferred embodiment, the protein is a human cytochrome P450 subfamily 3A selected from the group comprising CYP3A4 (SEQ ID N°11), CYP3A7 (SEQ ID N°15), CYP3A5 (SEQ ID N°12) and CYP3A43 (SEQ ID N°13). In still another preferred embodiment, the protein is a human cytochrome P450 3A4 or 3A7.
- Regarding the rebuilt P450 3A4 model, the main residues involved in the recognition of the substrate are C97; R104; F101; F107; F247; F303 and C376. More specifically, C97 and C376 are found in positions compatible with the formation of a disufide bridge allowing limited or enhanced flexibility of corresponding protein domains, while R104 is involved in the capture of the substrate that is close to the entrance site, and allows to accompany it to the active site. F303 is involved in the recognition of the substrate in the active site. F107; F247 and F303 are involved in the recognition at the modulation site responsible for positive regulation. Role of F303 in the active site has already been suggested by studies of Domanski et al. 1998 in the SRS 4 region (mutants I300, F303, A304, and T308).

Features of this model comprise the 3-D atomic coordinates of Table 3.

Table 3

In a preferred embodiment, the residues C97; R104; F101; F107; F247; F303 and C376 are involved in the CYP 3A4 for the recognition and uptake of the substrate at the entry site, and its binding into the active site having the 3-D atomic coordinates of Table 3.

Regarding the P450 3A7 model, features comprise the 3-D atomic coordinates of **Table 4**.

Table 4

In a preferred embodiment the residues Q79; F102; R105; R106; F108; F248; F304 and E374 are involved in the CYP 3A7 for the recognition and uptake of the substrate at the entry site, and its binding into the active having the 3-D atomic coordinates of Table 4.

In a third object, the invention contemplates a method for designing a protein, biological functions of which are altered, comprising:

- a) obtaining a 3-D model of said protein by the method as depicted above,
- b) analyzing said model of step a., and determining the amino-acids that are putatively involved in the biological functions of said protein,
 - c) changing said amino-acids by mutating the corresponding nucleotides on the nucleic acid sequence coding for said protein, in order to obtain a mutated protein having altered properties.

In the present invention, the term "altered properties" means that the generated protein is altered in its enzymatic properties, such as the substrate recognition, the movements associated to the entrance or the exit of the substrate, the multiple binding at the active site, the allosteric behaviour, the electron transfer, the coupling to the P450 reductase.

In another object, the invention relates to a computer-assisted method for performing restrained dynamics docking of a substrate on an enzyme, a 3-D structure of which is available, comprising the steps:

- j. determining a force field, and independently simulating the presence of said enzyme in said force field,
- k. minimizing the potential energy (Ep) linked to said force field of said 3-D structure, wherein the spatial position of some atoms of said enzyme is fixed, and wherein the other atoms are mobile, by allowing mobility of the mobile atoms, by i. simulating an increase in temperature (in order to give kinetic energy), ii. and minimizing the potential energy by re-specifying the temperature as 0 Kelvin (K)
- 30 I. optionally repeating step k in order to obtain other Ep minima, wherein said Ep minima are such that the structure of the protein remains folded,
 - m. minimizing Ep in said force field of said 3-D structure, wherein all the atoms of the protein are mobile, by

- i. simulating an increase in temperature (in order to give kinetic energy), and
- ii. minimizing the potential energy by re-specifying the temperature as 0 Kelvin (K)
- simulating, at 0 K the presence of said substrate next to said enzyme,
- optionally generating a molecular dynamics simulation on said substrate and 0. 5 enzyme (simulating an increase in temperature, in order to allow mobility of the atoms)
 - generating some constraints to said substrate, in order to impose that it has interaction with said enzyme,
- generating a molecular dynamics simulation on said substrate and enzyme, with said constraints imposed in step p., 10
 - optionally, generating a molecular dynamics simulation on said substrate and enzyme without said constraints of step p.

In the present invention, the term "restrained dynamics docking" means a procedure by which the docking of the substrate is simulated using molecular dynamics (MD) simulations under constraints that are specified by the user.

- In the present invention, the term "soft-restrained dynamics docking" refers to a restrained dynamics docking in which the substrate-protein distance constraints are loose, with force field parameters associated to the constraints as low as 1 or 2 Kcal/mol.
- 20 In the present invention, the term "constraints" when applied to substrate docking refers to a distance imposed between atoms of the protein, generally from the active site (such as atoms of the heme group), and atoms of the substrate. These distance restraints are defined as intervals, where the distance range is large enough to allow the free movement of the substrate within the active site.
- In a preferred embodiment of this method for performing restrained dynamics docking, said fixed atoms in step k. are the backbone atoms N-Ca-CO in the first minimization step and only Ca in subsequent minimization steps.

In another preferred embodiment of this method, kinetic energy is simulated by temperature increase to about 100 K for about 5-20 ns.

- The force field in step j. comprises forces linked to: 30
 - a. the distance between atoms,
 - b. the angles of valence,
 - c. the dihedral angles,

- d. the deformation with regard to planar geometry,
- e. the electrostatic field,
- f. the Van der Waals forces,
- g. hydrogen bonds.
- The constraints in step **p.** are attraction constraints to force said substrate in the active site, and wherein said constraints are not prejudiced to the exact spatial conformation of the substrate in the active site. These constraints are final distance constraints between some atoms of said substrate and some atoms of amino-acids present in said active site.
- In the present invention, the term "final distance constraints", when applied to substrate docking, means distances imposed between atoms from the heme group (such as the iron atom), and atoms of the substrate. These distance contraints are defined as intervals, and are related to the final position of the substrate in the vicinity of the heme group before metabolization.
- 15 Preferably, step o. is performed with a simulated temperature of between about 15 and 50 K, step q. is performed with a simulated temperature of between about 15 and 50 K, and step r. is performed with a simulated temperature of between about 200 and 350 K.
 - This method is particularly suited for multispecific protein such as a cytochrome 36 P450 subfamily 3A comprising mammal and human cytochromes.
 - The cytochrome can be cytochrome P450 3A4 or any of all other P450 from the 3A subfamily, and said structure can be the structure obtained by the method of the invention described above, in particular the model structures which atomic coordinates are listed in Tables 3 and 4 for CYP3A4 and CYP3A7.
- The substrate can be a small organic compound which size can range for example from MW 288 (testosterone) to MW 1203 (cyclosporine A).
 - In a preferred embodiment said substrate is testosterone.
 - In another object, the invention is aimed at a computer-assisted method for performing restrained dynamics docking of at least two substrates on an enzyme, a
 - 3-D structure of which is available, consisting of performing the steps j, k, l, m, n, o, p, q and r depicted above with a first substrate and repeating said steps with a second substrate when the first substrate reaches an unconstrained state after molecular dynamics simulations.

The first and second substrates can be the same molecule or different molecules.

The first and second substrates can display either allosteric or synergistic effect.

This method can be practiced with substrates that are inhibitors (competitive, uncompetitive, non competitive) or display an inhibitor-base mechanism. It can also

be practiced with an agonist and any molecule interfering with the biological function of the protein.

In preferred embodiments:

- the first and second substrates are the same molecule.
- the first and second substrates are different molecules.
- 10 the first and second substrates display an allosteric effect.
 - the first and second substrates display a synergistic effect.
 - at least one of the substrates is an inhibitor or display an inhibitor-based mechanism.
 - at least one of the substrates is an agonist.
- In another embodiment, this method also embraces a successive repeat of the steps j, k, l, m, n, o, p, q and r depicted above with a 3rd, 4th or 5th substrate, some of them being the same or different molecules.

In this method for performing restrained dynamics docking, said fixed atoms in step \mathbf{k} , are the backbone atoms N-C α -CO in the first minimization step and only C α in subsequent minimization steps.

In addition, kinetic energy is simulated by temperature increase to about 100 K for about 5-20 ns.

The force field in step j. comprises preferably forces linked to

- a. the distance between atoms,
- 25 b. the angles of valence,

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- c. the dihedral angles,
- d. the deformation with regard to planar geometry,
- e. the electrostatic field,
- f. the Van der Waals forces,
- 30 g. hydrogen bonds.

The constraints in step p. are preferable attraction constraints to force said substrate in the active site, and wherein said constraints are not prejudiced to the exact spatial conformation of the substrate in the active site. These constraints are final distance

constraints between some atoms of said substrate and some atoms of amino-acids present in said active site.

Preferably, step o. is performed with a simulated temperature of between about 15 and 50 K, step q. is performed with a simulated temperature of between about 15 and 50 K, and step r. is performed with a simulated temperature of between about 200 and 350 K.

This method is particularly suited for multispecific protein such as a cytochrome P450. The cytochrome can be cytochrome P450 3A4, or any of all other P450 of the 3A subfamily and said structure can be the structure obtained by the method of the invention described above, in particular the model structures which atomic coordinates are listed in Tables 3 and 4 for CYP3A4 and CYP3A7.

In a preferred embodiment:

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- said cytochrome is cytochrome P450 3A4, and said structure is the structure obtained by the above-described method, in particular the above-described model structure,
- said first and second substrates are small organic compounds which size can range from MW 288 (testosterone) to MW 1203 (cyclosporine A),
- said substrate is testosterone.

The invention is also directed to the use of the method for designing a 3-D model of a protein and to the computer-assisted method for performing restrained dynamics docking as mentioned above for screening, designing or identifying natural, unnatural substrates or substrate analogs, as well as inhibitors, activators or modulators of said enzyme.

Another object of the invention is the use of these methods for determining the effect of a first substrate on a second substrate, which can also be applied to pharmaceutical products.

The invention contemplates the use of these methods for determining the effect of a first bound testosterone molecule on the access of a second testosterone molecule as well as for determining the mutual effect of a testosterone molecule with alpha-

naphtoflavone (αNF) molecule.

The invention is also directed to:

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- * The use of the above described computer-assisted methods for determining the oxidative modification of the substrate according to the proximity to the heme of a part of the substrate to give rise to metabolite.
- The oxidized or reduced molecule derived from a given substrate modified after positioning at the right distance to the heme is called metabolite.

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- * The use of the above described computer-assisted methods, for performing dynamic docking of the said metabolite, either in the absence or in the presence of the second substrate in the calculation.
- * The use of the above described computer-assisted methods for dynamic docking to compare the energy of the bound metabolite relatively to the energy of its parent substrate bound, in order to determine if the exit of the given metabolite from the enzyme is favored or not.
 - * The use of the above described computer-assisted methods for dynamic docking to study the different exit pathways that are accessible to the metabolite, either in the absence or in the presence of the second substrate in the calculation.

The distance and angular constraints derived from CSBs common to the crystallized cytochromes P450 used as structural templates, are applied to conserved atoms of CSBs of the target protein. The DYANA software (Güntert et al. 1997) allows to rebuild directly the whole structure of the target protein on the basis of its primary sequence, by taking into account these geometric constraints. Out-of-blocks residues are rebuilt *ab initio* by selecting the most favorable solutions in terms of minimal global potential energy. As examples, actual tables 3 and 4 display the atomic coordinates of structural models obtained by applying DYANA calculation to target protein sequences CYP3A4 and CYP3A7 respectively.

```
TABLE 3 :Providing the coordinates of the CYP3A4 model
HEADER
          CYP3A4
          MODEL OF HUMAN CYTOCHROME P450 CYP3A4
TITLE
             LOISEAU, F. ANDRE, C. MINOLETTI, M. DELAFORGE
AUTHOR
                   SER TYR HIS LYS GLY PHE CYS MET PHE ASP MET GLU CYS
SEQRES
              452
                    HIS LYS LYS TYR GLY LYS VAL TRP GLY PHE TYR ASP GLY
SEORES
                    GLN GLN PRO VAL LEU ALA ILE THR ASP PRO ASP MET ILE
              452
SEORES
         3
                    LYS THR VAL LEU VAL LYS GLU CYS TYR SER VAL PHE THR
              452
SEQRES
         4
                    ASN ARG ARG PRO PHE GLY PRO VAL GLY PHE MET LYS SER
              452
SEQRES
         5
                    ALA ILE SER ILE ALA GLU ASP GLU GLU TRP LYS ARG LEU
SEQRES
         6
               452
                    ARG SER LEU LEU SER PRO THR PHE THR SER GLY LYS LEU
         7
               452
SEQRES
                    LYS GLU MET VAL PRO ILE ILE ALA GLN TYR GLY ASP VAL
SEQRES
         8
               452
                    LEU VAL ARG ASN LEU ARG ARG GLU ALA GLU THR GLY LYS
SEQRES
               452
                    PRO VAL THR LEU LYS ASP VAL PHE GLY ALA TYR SER MET
        10
               452
SEORES
                    ASP VAL ILE THR SER THR SER PHE GLY VAL ASN ILE ASP
               452
SEORES
        11
                    SER LEU ASN ASN PRO GLN ASP PRO PHE VAL GLU ASN THR
SEQRES
               452
        12
                    LYS LYS LEU LEU ARG PHE ASP PHE LEU ASP PRO PHE PHE
SEQRES
        13
               452
                    LEU SER ILE THR VAL PHE PRO PHE LEU ILE PRO ILE LEU
SEQRES
        14
               452
                    GLU VAL LEU ASN ILE CYS VAL PHE PRO ARG GLU VAL THR
        15
               452
SEQRES
                    ASN PHE LEU ARG LYS SER VAL LYS ARG MET LYS GLU SER
               452
SEQRES
        16
                    ARG LEU GLU ASP THR GLN LYS HIS ARG VAL ASP PHE LEU
               452
SEQRES
        17
                    GLN LEU MET ILE ASP SER GLN ASN SER LYS GLU THR GLU
SEORES
        18
               452
                    SER HIS LYS ALA LEU SER ASP LEU GLU LEU VAL ALA GLN
SEQRES
        19
               452
                    SER ILE ILE PHE ILE PHE ALA GLY TYR GLU THR THR SER
               452
        20
SEORES
                    SER VAL LEU SER PHE ILE MET TYR GLU LEU ALA THR HIS
               452
SEORES
        21
                    PRO ASP VAL GLN GLN LYS LEU GLN GLU GLU ILE ASP ALA
SEQRES
        22
               452
                    VAL LEU PRO ASN LYS ALA PRO PRO THR TYR ASP THR VAL
SEQRES
         23
               452
                    LEU GLN MET GLU TYR LEU ASP MET VAL VAL ASN GLU THR
SEQRES
         24
               452
                    LEU ARG LEU PHE PRO ILE ALA MET ARG LEU GLU ARG VAL
               452
SEQRES
         25
                    CYS LYS LYS ASP VAL GLU ILE ASN GLY MET PHE ILE PRO
SEQRES
         26
               452
                    LYS GLY TRP VAL VAL MET ILE PRO SER TYR ALA LEU HIS
         27
               452
SEORES
                    ARG ASP PRO LYS TYR TRP THR GLU PRO GLU LYS PHE LEU
SEQRES
               452
         28
                    PRO GLU ARG PHE SER LYS LYS ASN LYS ASP ASN ILE ASP
SEORES
         29
               452
                    PRO TYR ILE TYR THR PRO PHE GLY SER GLY PRO ARG ASN
SEQRES
         30
               452
                    CYS ILE GLY MET ARG PHE ALA LEU MET ASN MET LYS LEU
               452
SEORES
         31
                    ALA LEU ILE ARG VAL LEU GLN ASN PHE SER PHE LYS PRO
SEQRES
         32
               452
                    CYS LYS GLU THR GLN ILE PRO LEU LYS LEU SER LEU GLY
SEQRES
         33
               452
                    GLY LEU LEU GLN PRO GLU LYS PRO VAL VAL LEU LYS VAL
SEORES
         34
               452
                    GLU SER ARG ASP GLY THR VAL SER GLY ALA
SEQRES
         35
               452
               600
HET
HETNAM HEM
               HEME
               3,7,12,17-TETRAMETHYL-8,13-DIVINYL-2,18-PORPHINEDIPROPIONIC ACID
HETSYN HEM
               C34 H34 N4 O4 FE1
FORMUL HEM
                                   9.999 -1.760 -4.543 1.00
                                                                  0.00
                  SER
                          51
              N
MOTA
           1
                                                                  0.00
                                                                                3A4
                                                           1.00
                                                  -4.293
                                  10.718
                                           -0.477
                  SER
                          51
ATOM
           2
              CA
                                                                                3A4
                                                           1.00
                                                                  0.00
                                   9.949
                                            0.731
                                                   -4.939
                          51
MOTA
           3
              CB
                  SER
                                                                                3A4
                                                                  0.00
                                   8.601
                                            0.876
                                                   -4.493
                                                           1.00
MOTA
           4
              OG
                  SER
                          51
                                                                                3A4
                                                                  0.00
                                  10.962
                                           -0.281
                                                   -2.815
                                                           1.00
           5
              С
                   SER
                          51
MOTA
                                                                                3A4
                                                   -1.969
                                                            1.00
                                                                  0.00
                                           -0.855
                                  10.277
MOTA
              0
                   SER
                          51
                                                                                3A4
                                  11.974
                                                   -2.482
                                                            1.00
                                                                  0.00
                                           0.569
              N
                   TYR
                          52
ATOM
                                                                                3A4
                                                            1.00
                                                                  0.00
                                            0.860
                                                   -1.131
                          52
                                  12.433
           8
              CA
                  TYR
 MOTA
                                                                                3A4
                                                                  0.00
                                            0.783
                                                   -0.979
                                                            1.00
                          52
                                  13.983
              СВ
                  TYR
 ATOM
           9
                                                                  0.00
                                                                                3A4
                                                            1.00
                                           -0.572
                                                   -1.430
                                  14.459
                          52
          10
              CG
                   TYR
 ATOM
                                                                                3A4
                                           -1.732
                                                            1.00
                                                                  0.00
                                  14.143
                                                   -0.699
                          52
              CD1 TYR
 MOTA
          11
                                                            1.00
                                                                  0.00
                                                                                3A4
                                  15.210
                                           -0.701
                                                   -2.611
                          52
              CD2 TYR
 ATOM
          12
                                                                  0.00
                                                                                3A4
                                                            1.00
                                  14.574
                                           -2.994
                                                   -1.138
                          52
 ATOM
          13
              CE1 TYR
                                                                  0.00
                                                                                3A4
                                                            1.00
                                  15.651
                                           -1.954
                                                    -3.052
                          52
 MOTA
          14
              CE2 TYR
                                                                                3A4
                                                                  0.00
                                   15.334
                                           -3.105
                                                    -2.314
                                                            1.00
              CZ
                   TYR
                          52
 ATOM
          15
                                                                  0.00
                                                                                3A4
                                   15.784
                                           -4.370
                                                    -2.751
                                                            1.00
                   TYR
                          52
 MOTA
          16
              OH
                                                                                3A4
                                   11.971
                                                    -0.755
                                                            1.00
                                                                  0.00
                                            2.246
                          52
 ATOM
          17
              С
                   TYR
                                                            1.00
                                                                  0.00
                                                                                3A4
                                            3.208
                                                    -1.494
                                   12.178
 ATOM
          18
              ٥
                   TYR
                          52
                                                                                3A4
                                                            1.00
                                                                  0.00
                                            2.350
                                                     0.429
                   HIS
                          53
                                   11.321
 ATOM
              N
          19
                                                            1.00
                                                                   0.00
                                                                                3A4
                                                     0.953
                                   10.747
                                            3,568
                   HIS
                          53
              CA
 ATOM
          20
                                                                                 3A4
                                                            1.00
                                                                   0.00
                                                     1.039
              ND1 HIS
                          53
                                    7.857
                                            1.850
 MOTA
          21
                                                                                 3A4
                                                     0.097
                                                            1.00
                                                                   0.00
                                    8.485
                                            2.636
                          53
 ATOM
          22
              CG
                   HIS
                                                                                 3A4
                                                     0.386
                                                            1.00
                                                                   0.00
                                            3.861
                          53
                                    9.322
 ATOM
          23
              CB
                   HTS
                                                                   0.00
                                                                                 3A4
                                                            1.00
                                            0.923
                                                    -0.936
                                    7.438
                           53
 MOTA
          24
              NE2 HIS
                                                                   0.00
                                                                                 3A4
                                            2.053
                                                    -1.104
                                                            1.00
                                    8.216
          25
               CD2 HIS
                          53
 ATOM
                                                                                 3A4
                                                     0.368
                                                            1.00
                                                                   0.00
                                    7.247
                                            0.842
               CE1 HIS
                          53
 MOTA
          26
                                                                   0.00
                                                                                 3A4
                                   10.751
                                             3.386
                                                     2.448
                                                            1.00
                   HIS
                           53
          27
              C
 MOTA
                                                     3.080
                                                             1.00
                                                                   0.00
                                                                                 3A4
                                    9.715
                                             3.183
                           53
          28
              0
                   HIS
 MOTA
                                                                   0.00
                                                                                 344
                                                            1.00
                                                     3.043
           29
              N
                   LYS
                           54
                                   11.973
                                             3.461
 MOTA
```

ATOM	30	CA	LYS	54	12.265	3.262	4.451	1.00	0.00		3A4
MOTA	31	CB	LYS	54	13.401	2.217	4.659	1.00	0.00		3A4
MOTA	32	CG	LYS	54	13.053	0.819	4.120	1.00	0.00		3A4 3A4
MOTA	33	CD	LYS	54	14.220 14.793	-0.183 -0.500	4.148 5.540	1.00	0.00		3A4
MOTA	34 35	CE NZ	LYS	54 54	13.763	-1.087	6.431	1.00	0.00		3A4
ATOM ATOM	36	C	LYS	54	12.660	4.603	5.025	1.00	0.00		3A4
ATOM	37	ŏ	LYS	54	13.829	4.851	5.317	1.00	0.00		3A4
ATOM	38	N	GLY	55	11.656	5.510	5.181	1.00	0.00		3A4
ATOM	39	CA	GLY	55	11.819	6.901	5.560	1.00	0.00		3A4
ATOM	40	C	GLY	55 55	11.464	7.113	7.003 7.400	1.00	0.00		3A4 3A4
ATOM	41 42	О И	GLY PHE	55 56	10.305 12.502	7.002 7.439	7.817	1.00	0.00		3A4
ATOM ATOM	43	CA	PHE	56	12.451	7.714	9.250	1.00	0.00		3A4
ATOM	44	СВ	PHE	56	13.646	7.051	10.010	1.00	0.00		3A4
ATOM	45	CG	PHE	56	13.966	5.681	9.448	1.00	0.00		3A4
ATOM	46		PHE	56	15.250	5.415	8.926	1.00	0.00		3A4
ATOM	47		PHE	56	12.987	4.669	9.370 8.320	1.00	0.00		3A4 3A4
ATOM	48 49	CE1	PHE	56 56	15.543 13.271	4.185 3.445	8.747	1.00	0.00		3A4
ATOM ATOM	50	CZ	PHE	56	14.550	3.205	8.224	1.00	0.00		3A4
ATOM	51	c	PHE	56	12.446	9.211	9.542	1.00	0.00		3A4
ATOM	52	0	PHE	56	11.957	9.670	10.570	1.00	0.00	•	3A4
ATOM	53	N	CYS	57	12.971	10.054	8.624	1.00	0.00		3A4
ATOM	54	CA	CYS	57	13.048	11.500	8.782 7.665	1.00	0.00		3A4 3A4
ATOM	55	CB SG	CYS	57 57	13.902 15.312	12.161 11.121	7.176	1.00	0.00		3A4
ATOM ATOM	56 57	C	CYS	57	11.705	12.171	8.760	1.00	0.00		3A4
ATOM	58	ŏ	CYS	57	11.446	13.160	9.434	1.00	0.00		3A4
ATOM	59	N	MET	58	10.778	11.585	7.975	1.00	0.00		3A4
ATOM	60	CA	MET	58	9.402	12.000	7.870	1.00	0.00		3A4
MOTA	61	CB	MET	58	8.715 9.360	11.289	6.694 5.343	1.00	0.00		3A4 3A4
ATOM	62 63	CG SD	MET MET	58 58	8.469	11.641	3.887	1.00	0.00		3A4
ATOM ATOM	64 -	CE	MET	58	8.922	9.256	4.080	1.00	0.00		3A4
ATOM	65	c	MET	58	8.612	11.706	9.122	1.00	0.00		3A4
ATOM	66	0	MET	58	7.740	12.480	9.487	1.00	0.00		3A4
ATOM	67	N	PHE	59	8.963	10.612	9.844	1.00	0.00		3A4 3A4
ATOM	68	CA CB	PHE	59 59	8.394 8.732	10.230 8.752	11.122 11.449	1.00	0.00		3A4
ATOM ATOM	69 70	CG	PHE	59 ·	7.865	8.152	12.538	1.00	0.00		3A4
ATOM	71 .		PHE	59	6.477	8.002	12.350	1.00	0.00		3A4
ATOM	72	CD2	PHE	59	8.430	7.747	13.764	1.00	0.00		3A4
· ATOM	73	CE1		59	5.671	7.462	13.364	1.00	0.00		3A4 3A4
MOTA	74		PHE	59	7.627	7.208	14.780 14.579	1.00	0.00		3A4
ATOM	75 76	CZ	PHE	59 · 59	6.247 8.881	7.065 11.119	12.255	1.00	0.00		3A4
ATOM ATOM	77	0	PHE	59	8.110	11.479	13.139	1.00	0.00		3A4
ATOM	78	N	ASP	60	10.162	11.568	12.226	1.00	0.00		3A4
ATOM	79	CA	ASP	60	10.690	12.515	13.200	1.00	0.00	•	3A4
MOTA	80	CB	ASP	60	12.225	12.651	13.131	1.00	0.00		3A4 3A4
ATOM	81	CG	ASP	60	12.906 12.613	11.313 10.736	13.450 14.532	1.00	0.00		3A4
ATOM ATOM	82 83		ASP ASP	60 60	13.743	10.750	12.624	1.00	0.00		3A4
ATOM	84	C	ASP	60	10.102	13.900	13.031	1.00	0.00		3A4
ATOM	85	0	ASP	60	9.841	14.603	14.000	1.00	0.00		3A4
ATOM	86	N	MET	61	9.809	14.318	11.780	1.00	0.00		3A4
ATOM	87	CA	MET	61	9.130	15.564	11.481 9.987	1.00	0.00		3A4 3A4
ATOM.	88 89	CB CG	MET MET	61 61	9.224 10.590	15.881 16.349	9.497	1.00	0.00		3A4
ATOM ATOM	90	SD	MET	61	10.659	16.502	7.686	1.00	0.00		3A4
ATOM	91	CE	MET	61	12.223	17.411	7.689	1.00	0.00		3A4
ATOM	92	c	MET	61	7.653	15.548	11.870	1.00	0.00		3A4
ATOM	93	0	MET	61	7.073	16.551	12.274	1.00	0.00		3A4
MOTA	94	N	GLU	62	7.012	14.358	11.819	1.00	0.00		3A4 3A4
ATOM	95 96	CA	GLU	62 62	5.653 5.077	14.159 · 12.770	12.272	1.00	0.00		3A4
ATOM ATOM	96 97	CB	GLU	62	4.640	12.657	10.462	1.00	0.00		3A4
ATOM	98	CD	GLU	62	4.351	11.190	10.120	1.00	0.00		3A4
ATOM	99		GLU	62	3.429	10.603	10.748	1.00	0.00		3A4
ATOM	100		GLU	62	5.048	10.637	9.227	1.00	0.00		3A4
ATOM	101	С	GLU	62	5.522	14.338	13.751	1.00	0.00		3A4

MOTA	102	0	GLU	62	4.508	14.819	14.225	1.00	0.00	3A4
ATOM	103	N	CYS	63	6.605	14.104	14.522	1.00	0.00	3A4 3A4
MOTA	104	CA	CYS	63	6.664 7.902	14.441 13.805	15.921 16.588	1.00	0.00	3A4
MOTA MOTA	105 106	CB SG	CYS	63 63	7.977	11.995	16.382	1.00	0.00	3A4
ATOM	107	c	CYS	63	6.526	15.952	16.211	1.00	0.00	3A4
MOTA	108	0	CYS	63	6.277	16.322	17.335	1.00	0.00	3A4
MOTA	109	N	HIS	64	6.436	16.853	15.182	1.00	0.00	3A4 3A4
MOTA	110 111	CA	HIS	64 64	5.487 4.140	17.970 20.440	15.236 16.744	1.00	0.00	3A4
ATOM ATOM	112	CG	HIS	64	5.232	20.460	15.904	1.00	0.00	3A4
ATOM	113	CB	HIS	64	6.151	19.284	15.666	1.00	0.00	3A4
MOTA	114		HIS	64	4.280	22.506	15.939	1.00	0.00	3A4 3A4
ATOM ATOM	115 116		HIS HIS	64 64	5.301 3.608	21.731 21.687	15.420 16.726	1.00	0.00	3A4
ATOM	117	C	HIS	64	4.780	18.138	13.901	1.00	0.00	3A4
ATOM	118	0	HIS	64	3.812	17.438	13.610	1.00	0.00	3A4
MOTA	119	N '	LYS	65	5.240	19.107	13.073 11.766	1.00	0.00	3A4 3A4
ATOM	120 121	CA CB	LYS LYS	65 65	4.699 3.264	19.426 20.052	11.761	1.00	0.00	3A4
ATOM ATOM	122	CG	LYS	65	2.994	21.171	12.783	1.00	0.00	3A4
ATOM	123	CD	LYS	65	1.557	21.704	12.722	1.00	0.00	3A4
MOTA	124	CE	LYS	65	1.220	22.723	13.820	1.00	0.00	3A4 3A4
ATOM	125 126	NZ C	LYS LYS	65 65	2.052 5.705	23.944 20.365	13.700 11.146	1.00	0.00	3A4
ATOM ATOM	127	ŏ	LYS	65	5.958	20.315	9.944	1.00	0.00	3A4
ATOM	128	N	LYS	66	6.332	21.227	12.000	1.00	0.00	3A4
MOTA	129	CA	LYS	66	7.517	22.020	11.730 12.037	1.00	0.00	3A4 3A4
ATOM	130 131	CB CG	LYS LYS	66 66	7.373 6.519	23.548 24.352	11.039	1.00	0.00	3A4
MOTA MOTA	132	CD	LYS	66	5.001	24.175	11.175	1.00	0.00	3A4
ATOM	133	CE	LYS	66	4.191	25.119	10.278	1.00	0.00	3A4
MOTA	134	NZ	LYS	66	2.736	24.881	10.442	1.00	0.00	3A4 3A4
ATOM	135 136	С 0	LYS LYS	66 66	8.551 9.100	21.370 20.332	12.620 12.253	1.00	0.00	3A4
MOTA MOTA	137	N	TYR	67	8.772	21.934	13.838	1.00	0.00	3A4
ATOM	138	CA	TYR	67	9.441	21.263	14.936	1.00	0.00	3A4
MOTA	139	СВ	TYR	67	11.005	21.348	14.926	1.00	0.00	3A4 3A4
MOTA MOTA	140 141	CG	TYR TYR	67 67	11.555 11.325	20.265 18.909	14.028 14.336	1.00	0.00	3A4
ATOM	142		TYR	67	12.250	20.569	12.847	1.00	0.00	3A4
ATOM	143		TYR	67	11.798	17.884	13.506	1.00	0.00	3A4
ATOM	144		TYR	67	12.720	19.550	12.006 12.342	1.00	0.00	. 3A4 3A4
MOTA MOTA	145 146	CZ- OH	TYR TYR	67 67	12.507 13.010	18.207 17.184	11.509	1.00	0.00	3A4
ATOM	147	C	TYR	67	8.880	21.880	16.194	1.00	0.00	3A4
ATOM	148	0	TYR	67	8.905	23.092	16.404	1.00	0.00	3A4
MOTA	149	N	GLY	68 ·	8.343	20.969	17.043 18.278	1.00	0.00	3A4 3A4
MOTA MOTA	150 151	CA	GLY GLY	68 68	7.620 8.251	20.139	19.164	1.00	000	3A4
ATOM	152	ŏ	GLY	68	8.314	18.954	18.839	1.00	0.00	3A4
ATOM	153	N	LYS	69	8.864	20.642	20.260	1.00	0.00	3A4 3A4
ATOM	154	CA	LYS	69 60	10.301 10.795	20.592 21.997	20.404 20.802	1.00	0.00	3A4 3A4
ATOM ATOM	155 156	CB CG	LYS	69 69	10.733	23.112	19.844	1.00	0.00	3A4
ATOM	157	CD	LYS	69	10.770	24.527	20.225	1.00	0.00	3A4
MOTA	158	CE	LYS	69	9.876	25.161	21.300	1.00	0.00	3A4 3A4
ATOM	159	NZ	LYS	69 69	10.236 10.811	26.582 19.541	21.514 21.360	1.00	0.00	3A4
ATOM ATOM	160 161	с 0	LYS LYS	69	11.914	19.033	21.177	1.00	0.00	3A4
ATOM	162	N	VAL	70	10.033	19.200	22.410	1.00	0.00	3A4
ATOM	163	CA	VAL	70	10.427	18.227	23.408	1.00	0.00	3A4 3A4
ATOM	164 165	CB CG1	VAL VAL	70 70	10.984 12.504	18.837 18.835	24.696 24.571	1.00	0.00	3A4
ATOM ATOM	166		VAL	70 70	10.344	20.206	25.037	1.00	0.00	3A4
MOTA	167	C	VAL	70	9.212	17.394	23.695	1.00	0.00	3A4
ATOM	168	0	VAL	70	8.176	17.901	24.111	1.00	0.00	3A4 3A4
MOTA	169	N CA	TRP TRP	71 71	9.337 8.255	16.067 15.133	23.484 23.636	1.00	0.00	3A4
ATOM ATOM	170 171	CB	TRP	71	7.614	14.787	22.260	_	0.00	3A4
ATOM	172	CG	TRP	71	6.390	13.874	22.229	1.00	0.00	3A4
MOTA	173	CD2	TRP	71	5.135	14.145	22.880	1.00	0.00	3A4

ATOM	174	CD1	TRP	71	6.251	12.660	21.615	1.00	0.00		3A4
MOTA	175	NE1	TRP	71	4.996	12.146	21.846	1.00	0.00		3A4
ATOM	176	CE2	TRP TRP	71 71	4.292 4.695	13.040 15.227	22.624 23.643	1.00	0.00		3A4 3A4
ATOM ATOM	177 178		TRP	71	2.995	12.995	23.131	1.00	0.00		3A4
ATOM	179		TRP	71	3.388	15.180	24.153	1.00	0.00		3A4
MOTA	180	CH2	TRP	71	2.551	14.080	23.902	1.00	0.00		3A4
MOTA	181	C	TRP	71	8.828	13.911	24.261	1.00	0.00		3A4 3A4
ATOM ATOM	182 183	O N	TRP	71 72	9.989 7.987	13.584 13.188	24.059 25.027	1.00	0.00		3A4
ATOM	184	CA	GLY	72	8.345	11.936	25.647	1.00	0.00		3A4
ATOM	185	C	GLY	72	7.812	10.809	24.804	1.00	0.00		3A4
ATOM	186	0	GLY	72	6.679	10.850	24.336	1.00	0.00		3A4
ATOM ATOM	187	N	PHE	73 73	8.645 8.334	9.773 8.591	24.586 23.820	1.00	0.00		3A4 3A4
ATOM	188 189	CA CB	PHE	73	9.278	8.443	22.586	1.00	0.00		3A4
ATOM	190	CG	PHE	73	8.893	7.320	21.647	1.00	0.00		3A4
ATOM	191		PHE	73	9.691	6.162	21.549	1.00	0.00		3A4
ATOM	192		PHE	73	7.717	7.398	20.877	1.00	0.00		3A4 3A4
ATOM ATOM	193 · 194	CE1	PHE	73 73	9.320 7.344	5.105 6.343	20.707	1.00	0.00		3A4
MOTA	195	CZ	PHE	73	8.146	5.196	19.947	1.00	0.00		3A4
ATOM	196	C	PHE	73	8.515	7.451	24.788	1.00	0.00		3A4
MOTA	197	0	PHE	73	9.257	7.543	25.757	1.00	0.00		3A4
ATOM	198	N	TYR	74	7.826	6.328	24.540 25.397	1.00	0.00		3A4 3A4
MOTA MOTA	199 200	CA CB	TYR TYR	74 74	7.884 6.631	5.174 5.032	26.304	1.00	0.00		3A4
ATOM	201	CG	TYR	74	5.298	5.291	25.625	1.00	0.00		3A4
ATOM	202	CD1	TYR	74	4.515	4.223	25.146	1.00	0.00		3A4
MOTA	203		TYR	74	4.797	6.603	25.491	1.00	0.00		3A4
ATOM ATOM	204 205	CE1	TYR TYR	74 74	3.279 3.564	4.456 6.844	24.524 24.870	1.00	0.00		3A4 3A4
ATOM	206	CZ	TYR		2.804	5.769	24.384	1.00	0.00		3A4
ATOM	207	OH	TYR	74	1.560	6.006	23.757	1.00	0.00		3A4
MOTA	208	C	TYR	74	8.100	4.007	24.486	1.00	0.00		3A4
ATOM	209	0	TYR	74 .	7.256	3.682	23.658	1.00	0.00	•	3A4 3A4
ATOM ATOM	210 211	N CA	ASP ASP	75 75	9.272 9.664	3.357 2.238	24.603 23.778	1.00	0.00		3A4
ATOM	212	СВ	ASP	75	11.110	2.479	23.220	1.00	0.00		3A4
ATOM	213	CG	ASP	75 .	11.483	1.556	22.044	1.00	0.00		3A4
ATOM	214		ASP	75 ·	10.755	1.577	21.015	1.00	0.00		3A4
ATOM ATOM	215 216	C C	ASP ASP	75 75	12.500 9.580	0.822 1.007	22.166 24.657	1.00	0.00		3A4 3A4
ATOM	217	.0	ASP	75	9.275	1.091	25.845	1.00	0.00		3A4
MOTA	218	N	GLY	76	9.925	-0.191	24.123	1.00	0.00		3A4
MOTA	219	CA	GLY	76	10.101	-1.403	24.908	1.00	0.00		3A4
ATOM	220	C	GLY	· 76 76	11.420 12.463	-1.335 -1.562	25.643 25.039	1.00	0.00		3A4 3A4
ATOM ATOM	221 222	O N	GLY	77	11.349	-0.928	26.946	1.00	0.00		3A4
ATOM	223	CA	GLN	. 77	12.393	-0.521	27.882	1.00	0.00		3A4
MOTA	224	СВ	GLN	77	13.760	-1.300	27.835	1.00	0.00		3A4
ATOM	225	CG	GLN	77	14.891	-0.783	26.903	1.00	0.00		3A4 3A4
ATOM ATOM	226 227	CD OE1	GLN GLN	77 77	15.977 16.121	-1.843 -2.718	26.760 27.611	1.00	0.00		3A4
MOTA	228	NE2		77	16.759	-1.765	25.648	1.00	0.00		3A4
ATOM	229	С	GLN	77	12.593	0.983	27.782	1.00	0.00		3A4
ATOM	230	0	GLN	77	12.935	1.504	26.719	1.00	0.00		3A4
ATOM ATOM	231 232	N CA	GLN GLN	78 78	12.365 12.698	1.707 3.105	28.918 29.188	1.00	0.00		3A4 3A4
ATOM	232	CB	GLN	78	14.220	3.411	28.944	1.00	0.00		3A4
ATOM	234	CG	GLN	78	14.774	4.789	29.381	1.00	0.00		3A4
ATOM	235	CD	GLN	78	14.622	5.043	30.889	1.00	0.00		3A4
ATOM	236	OE1		78 70	14.409	4.138	31.694	1.00	0.00		3A4 3A4
ATOM ATOM	237 238	NE2 C	GLN	78 78	14.757 11.820	6.336 4.135	31.296 28.453	1.00	0.00		3A4 3A4
ATOM	239	ŏ	GLN	78	11.794	4.125	27.222	1.00	0.00		3A4
MOTA	240	N	PRO	79	11.120	5.089	29.129	1.00	0.00		3A4
ATOM	241	CA	PRO	79	10.604	6.330	28.550	1.00	0.00		3A4
ATOM ATOM	242 243	CD CB	PRO PRO	79 79	10.730 9.535	4.946 6.798	30.533 29.557	1.00	0.00		3A4 3A4
ATOM	243	CG	PRO	79 79	10.001	6.244	30.911	1.00	0.00		3A4
ATOM	245	c	PRO	79	11.734	7.327	28.383	1.00	0.00		3A4

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ATOM	246	0	PRO	79	12.582	7.447	29.260	1.00	0.00	37	44
ATOM	247	N	VAL	80	11.782	8.012	27.228	1.00	0.00	37	
ATOM	248	CA	VAL	80	12.870	8.876	26.835	1.00	0.00	37	
MOTA	249	CB	VAL	80	13.698	8.283	25.679 26.173	1.00	0.00	37 37	
MOTA MOTA	250 251		VAL VAL	80 80	14.441 12.828	7.026 7.928	24.440	1.00	0.00	37	
MOTA	252	C	VAL	80	12.250	10.173	26.392	1.00	0.00	37	
ATOM	253	ō	VAL	80	11.117	10.204	25.939	1.00	0.00	37	
MOTA	254	N	LEU	81	13.003	11.285	26.466	1.00	0.00		A4
ATOM	255	CA	LEU	81	12.603	12.575	25.948	1.00	0.00		A4 A4
ATOM	256 257	CB CG	LEU	81 81	12.958 12.302	13.700 15.079	26.945 26.699	1.00	0.00		A4
MOTA MOTA	258		LEU	81	10.822	15.078	27.116	1.00	0.00		A4
ATOM	259		LEU	81	13.057	16.197	27.437	1.00	0.00	37	A4
ATOM	260	¢	LEU	81	13.352	12.751	24.647	1.00	0.00		A4
MOTA	261	0	LEU	81	14.529	12.427	24.569	1.00	0.00		A4 A4
MOTA	262	И	ALA	82 82	12.695 13.260	13.249 13.415	23.585 22.267	1.00	0.00		A4
MOTA MOTA	263 264	CA CB	ALA	82	12.433	12.689	21.183	1.00	0.00		A4
ATOM	265	c	ALA	82	13.288	14.890	21.990	1.00	0.00	32	A4
ATOM	266	ο.	ALA	82	12.251	15.546	22.002	1.00	0.00		A4
MOTA	267	N	ILE	83	14.498	15.436	21.733	1.00	0.00		A4
ATOM	268	CA	ILE	83	14.742 16.032	16.837 17.330	21.486 22.124	1.00	0.00		A4 A4
ATOM ATOM	269 270	CB CG2	ILE	83 83	15.944	18.846	22.217	1.00	0.00		A4
ATOM	271	CG1	ILE	83	16.359	16.727	23.506	1.00	0.00	3	A4
ATOM	272	CD	ILE	83	15.380	17.044	24.634	1.00	0.00		A4
MOTA	273	C	ILE	83	14.831	17.000	19.986	1.00	0.00		A4 A4
ATOM	274	0	ILE	83 84	15.706 13.915	16.418 17.773	19.358 19.367	1.00	0.00		A4
ATOM ATOM	275 276	N CA	THR	84	13.796	17.851	17.920	1.00	0.00		A4
ATOM	277	СВ	THR	84	12.384	17.503	17.457	1.00	0.00	3:	A4
MOTA	278		THR	84	11.371	18.330	18.025	1.00	0.00		A4
MOTA	279		THR	84	12.085	16.027	17.808	1.00	0.00		A4
ATOM	280	C	THR	84	14.259 14.500	19.175 19.282	17.344 16.144	1.00	0.00		A4 A4
ATOM ATOM	281 282	0 N	THR	84 - 85	14.371	20.231	18.176	1.00	0.00		A4
ATOM	283	CA	ASP	85	14.595	21.594	17.732	1.00	0.00	3.	A4
ATOM	284	CB	ASP	85	13.703	22.550	18.577	1.00	0.00		A4
ATOM	285	CG	ASP	85	13.371	23.873	17.872	1.00	0.00		A4 A4
ATOM	286 287		ASP ASP	85 85	12.666 13.808	23.828 24.942	16.828 18.373	1.00	0.00		A4
MOTA MOTA	288	C	ASP	85	16.050	21.928	17.888	1.00	0.00		A4
ATOM	289	ō	ASP	85	16.660	21.452	18.843	1.00	0.00		A4
ATOM	290	N	PRO	86	16.683	22.732	17.024	1.00	0.00		A4
ATOM	291	CA	PRO	86	18.101	23.035	17.076 15.807	1.00	0.00		A4 A4
ATOM ATOM	· 292 293	CD CB	PRO PRO	86 86	16.102 18.421	23.257 23.751	15.747	1.00	0.00		A4
ATOM	294	CG	PRO	86	17.079	24.309	15.294	1.00	0.00		A4
ATOM	295	С	PRO	86	18.425	23.863	18.284	1.00	0.00		A4
ATOM	296	0	PRO	86	19.466	23.647	18.892	1.00	0.00		A4
ATOM	297	N	ASP	87	17.511 17.636	24.756 25.559	18.711 19.902	1.00	0.00		A4
MOTA MOTA	298 299	CA CB	ASP ASP	87 87	16.417	26.494	20.029	1.00	0.00	_	A4
ATOM	300	CG	ASP	87	16.305	27.442	18.820	1.00	0.00		A4
MOTA	301		ASP	87	17.357	27.851	18.258	1.00	0.00		A4
ATOM	302		ASP	87	15.148	27.764	18.439	1.00	0.00		A4
ATOM ATOM	303 304	C O	ASP ASP	87 87	17.724 18.546	24.745 25.018	21.171 22.032	1.00	0.00		A4
ATOM	305	N	MET	88	16.902	23.678	21.253	1.00	0.00		A4
ATOM	306	CA	MET	88	16.847	22.776	22.375	1.00	0.00		A4
ATOM	307	СВ	MET	88	15.536	22.000	22.396	1.00	0.00		A4
ATOM	308	CG	MET	88	14.362	22.948 22.177	22.644 23.469	1.00	0.00		BA4 BA4
ATOM ATOM	309 310	SD CE	MET MET	88 88	12.947 13.722	21.914	25.087	1.00	0.00		BA4
ATOM	311	C	MET	88	18.007	21.812	22.436	1.00	0.00	3	3A4
ATOM	312	0	MET	88	18.524	21.506	23.506	1.00	0.00		3A4
ATOM	313	N	ILE	89	18.500	21.349	21.264	1.00	0.00		3A4 3A4
ATOM	314	CA CB	ILE	89 89	19.637 19.679	20.450 19.800	21.170 19.793	1.00	0.00		3A4
ATOM ATOM	315 316		ILE	89	21.088	19.217	19.442	1.00	0.00		3A4
ATOM	317		ILE	89	18.596	18.681	19.910	1.00	0.00	3	3A4

ATOM	318	CD	ILE	89	18.390	17.678	18.773	1.00	0.00	3A4
ATOM	319	C	ILE	89	20.916	21.161	21.538	1.00	0.00	3A4
MOTA	320	0	ILE	89	21.722	20.655	22.310	1.00	0.00	3A4
MOTA	321	N	LYS	90	21.096 22.214	22.421 23.250	21.089 21.481	1.00	0.00	3A4 3A4
MOTA MOTA	322 323	CA CB	LYS LYS	90 9 0	22.225	24.577	20.719	1.00	0.00	3A4
MOTA	324	CG	LYS	90	23.531	25.387	20.790	1.00	0.00	3A4
ATOM	325	CD	LYS	90	23.546	26.569	19.811	1.00	0.00	3A4
ATOM	326	CE	LY\$	90	24.875	27.339	19.774	1.00	0.00	3A4
MOTA	327	NZ	LYS	90	25.167	27.975	21.082	1.00	0.00	3A4 3A4
MOTA	328	c	LYS LYS	90 90	22.221 23.248	23.564 23.567	22.961 23.612	1.00	0.00	3A4
MOTA MOTA	329 330	и О	THR	91	21.031	23.752	23.561	1.00	0.00	3A4
ATOM	331	CA	THR	91	20.855	23.981	24.981	1.00	0.00	3A4
ATOM	332	CB	THR	91	19.434	24.380	25.293	1.00	0.00	3A4
MOTA	333		THR	91	19.170	25.637	24.681	1.00	0.00	3A4 3A4
ATOM	334		THR	91 91	19.109 21.198	24.554 22.782	26.810 25.817	1.00	0.00 0.00	3A4
ATOM ATOM	335 336	С 0	THR	91	21.150	22.889	26.851	1.00	0.00	3A4
ATOM	337	N	VAL	92	20.849	21.578	25.307	1.00	0.00	3A4
ATOM	338	CA	VAL	92	21.125	20.315	25.945	1.00	0.00	3A4
MOTA	339	ÇВ	VAL	92	20.299	19.178	25.353	1.00	0.00	3A4
MOTA	340		VAL	92	21.025	18.247	24.370 26.498	1.00	0.00	3A4 3A4
MOTA	341		VAL	92 92 -	19.643 22.600	18.370 20.047	26.498	1.00	0.00	3A4
MOTA MOTA	342 343	C O	VAL	92 -	22.991	19.412	27.041	1.00	0.00	3A4
ATOM	344	N	LEU	93	23.483	20.706	25.311	1.00	0.00	3A4
ATOM	345	CA	LEU	93	24.914	20.851	25.543	1.00	0.00	3A4
ATOM	346	СВ	LEU	93	25.432	21.742	24.407	1.00	0.00	3A4 3A4
ATOM	347	CG	LEU	93 93	26.456 25.796	21.108 19.892	23.525 22.820	1.00	0.00	3A4
ATOM ATOM	348 349		LEU	93	26.955	22.238	22.601	1.00	0.00	3A4
ATOM	350	c	LEU	93	25.419	21.473	26.847	1.00	0.00	3A4
MOTA	351	0	LEU	93	24.654	21.997	27.655	1.00	0.00	3A4
ATOM	352	N	VAL	94	26.774	21.385	27.035	1.00	0.00	3A4 3A4
MOTA	353	CA	VAL	94 94	27.599 27.328	21.729 23.082	28.196 28.879	1.00	0.00	3A4
ATOM ATOM	354 355		VAL	. 94	28.368	23.358	30.001	1.00	0.00	
ATOM	356		VAL	94	27.427	24.201	27.813	1.00	0.00	. 3A4
MOTA	357	С	VAL	94	27.515	20.540	29.137	1.00	0.00	3A4
ATOM	358	0	VAL	94	26.875	20.578	30.188	1.00	0.00	3A4 3A4
ATOM	359	N	LYS LYS	95 95	28.141 28.019	19.421 18.101	28.690 29.261	1.00	0.00	3A4
ATOM ATOM	360 361	CA CB	LYS	95	27.404	17.078	28.259	1.00	0.00	3A4
ATOM	362	CG	LYS	95	27.757	17.284	26.778	1.00	0.00	3A4
MOTA	363	CD	LYS	95	27.133	16.199	25.898	1.00	0.00	3A4
ATOM	364	CE	LYS	95	27.017	16.559	24.413	1.00	0.00	3A4 3A4
MOTA	365 366	NZ C	LYS	95 95	28.338 29.379	16.819 17.675	23.809	1.00	0.00	3A4
ATOM ATOM	367	Ö	LYS	95	30.123	16.990	29.040	1.00	0.00	3A4
ATOM	368	N	GLU	96	29.703	18.085	30.988	1.00	0.00	3A4
ATOM	369	CA	GLU	96	30.926	17.783	31.698	1.00	0.00	3A4
MOTA	370.	CB	GLU	96	31.795	19.051	31.950	1.00	0.00	3A4 3A4
ATOM ATOM	371 372	CD	GLU	96 96	31.039 32.012	20.290	32.48.6 32.599	1.00	0.00	3A4
ATOM	373		GLU	96	31.790		31.901	1.00	0.00	3A4
ATOM	374		GLU	96	32.990	21.357	33.388	1.00	0.00	3A4
MOTA	375	С	GLU	96	30.517	17.078	32.969	1.00	0.00	3A4
MOTA	376	0	GLU	96 97	30.732 29.924	17.576 15.869	34.073 32.763	1.00	0.00	3A4 3A4
ATOM ATOM	377 378	N CA	CYS CYS	97 97	29.924	14.865	33.693	1.00	0.00	3A4
MOTA	379	CB	CYS	97	29.558	15.141	35.235	1.00	0.00	3A4
ATOM	380	SG	CYS	97	29.186	13.706	36.313	1.00	0.00	3A4
MOTA	381	С	CYS	97	28.000	14.633	33.277	1.00	0.00	3A4
MOTA	382	0	CYS	97 98	27.076 27.817	15.253 13.703	33.800 32.305	1.00	0.00	3A4 3A4
MOTA MOTA	383 384	N CA	TYR TYR		26.556	13.703	31.782	1.00	0.00	3A4
ATOM	385	CB	TYR		26.197	13.814	30.380	1.00	0.00	3A4
ATOM	386	CG	TYR	98	25.205	14.939	30.543	1.00	0.00	3A4
ATOM	387		TYR		25.573	16.198	31,050	1.00	0.00	3A4 3A4
MOTA MOTA	388 389		TYR TYR		23.862 24.626	14.731 17.224	30.197 31.198	1.00	0.00	3A4
ALUM	בסב	UELL	* 1 4	20	23.020					

ATOM	390	CE2	TYR	98	22.901	15.740	30.351	1.00	0.00	3A4	
ATOM	391	CZ	TYR	98	23.286	16.993	30.849	1.00	0.00	3A4	
ATOM	392	OH	TYR	98	22.323	18.015	30.999	1.00	0.00	3A4	
ATOM	393	C	TYR	98	26.800	11.735	31.683 30.891	1.00	0.00	3A4 3A4	
ATOM ATOM	394 395	O N	TYR SER	98 99	27.629 26.097	11.292 10.928	32.531	1.00	0.00	3A4	
ATOM	396	CA	SER	99	26.414	9.536	32.838	1.00	0.00	3A4	
ATOM	397	СВ	SER	99	25.870	9.141	34.247	1.00	0.00	3A4	
ATOM	398	OG	SER	99	26.515	7.992	34.791	1.00	0.00	3A4	
ATOM	399	С	SER	99	25.931	8.568	31.771	1.00	0.00	3A4	
ATOM	400	0	SER	99	24.885	8.764 7.507	31.156 31.524	1.00	0.00	3A4 3A4	
MOTA	401 402	N CA	VAL VAL	100 100	26.759 26.647	6.426	30.542	1.00	0.00	3A4	
ATOM ATOM	403	CB	VAL	100	25.344	5.612	30.576	1.00	0.00	3A4	
ATOM	404		VAL	100	25.483	4.356	29.677	1.00	0.00	3A4	
MOTA	405	CG2	VAL	100	25.062	5.167	32.031	1.00	0.00	3A4	
ATOM	406	C	VAL	100	26.977	6.962	29.152	1.00	0.00	3A4 3A4	
ATOM	407	0	VAL	100	28.088 26.002	6.758 7.682	28.673 28.517	1.00	0.00	3A4	
ATOM ATOM	408 409	N CA	PHE PHE	101 101	26.131	8.581	27.372	1.00	0.00	3A4	
ATOM	410	СВ	PHE	101	27.487	9.383	27.359	1.00	0.00	3A4	1
ATOM	411	CG	PHE	101	27.503	10.546	26.402	1.00	0.00	3A4	
ATOM	412		PHE	101	26.587	11.609	26.522	1.00	0.00	3A4	
ATOM	413		PHE	101	28.432	10.563	25.350	1.00	0.00	3A4 3A4	
ATOM	414		PHE	101 101	26.580 28.435	12.640 11.597	25.573 24.418	1.00	0.00	3A4	
ATOM ATOM	415 416	CZ	PHE PHE	101	27.492	12.629	24.516	1.00	0.00	3A4	
ATOM	417	c	PHE	101	25.860	7.863	26.049	1.00	0.00	3A4	4
ATOM	418	0	PHE		25.613	8.506	25.030	1.00	0.00	3A4	
ATOM	419	N	THR	102	25.881	6.507	26.048	1.00	0.00	3A4	
MOTA	420	CA	THR	102	25.468	5.674 5.456	24.939 23.875	1.00	0.00	3A4 3A4	
ATOM ATOM	421 422	CB OG1	THR	102 102	26.561 26.134	4.618	22.803	1.00	0.00	3A4	
ATOM	423		THR	102	27.920	4.971	24.441	1.00	0.00	ЗА	
ATOM	424	c	THR	102	24.949	4.448	25.660	1.00	0.00	. 3A	
ATOM	425	0	THR	102	25.680	3.511	25.976	1.00	0.00	3A-	
MOTA	426	N	ASN	103	23.629	4.491	25.991	1.00	0.00	3A- 3A-	
ATOM	427	CA	ASN	103 103	22.973 22.145	3.634 4.482	26.965 28.000	1.00 1.00	0.00	3A	
ATOM ATOM	428 429	CB CG	ASN ASN	103	21.193	5.519	27.373	1.00	0.00	ЗА	
ATOM	430		ASN	103	21.530	6.702	27.345	1.00	0.00	3A:	4
ATOM	431		ASN	103	19.993	5.093	26.893	1.00	0.00	3A	
ATOM	432	С	ASN	103	22.171	2.529	26.295	1.00	0.00	3A 3A	
ATOM	433	0	ASN	103	22.526 21.099	2.061 2.084	25.214 27.018	1.00	0.00	3A	
ATOM ATOM	434 435	N CA	ARG ARG	·104 104	20.255	0.904	26.922	1.00	0.00	3A	
ATOM	436	СВ	ARG	104	20.057	0.305	25.521	1.00	0.00	. ЗА	4
ATOM .	437	CG	ARG	104	19.266	1.224	24.571	1.00	0.00	3A	
ATOM	438	CD	ARG	104	19.318		23.096	1.00	0.00	. 3A	
ATOM	439	NE	ARG	104	20.722	1.001	22.589 21.280	1.00	0.00	3A 3A	
MOTA	440 441	CZ NU1	ARG ARG	104 104	21.086 22.383	0.812 1.027	20.912	1.00	0.00	3A	
ATOM ATOM	442		ARG	104	20.184	0.403	20.340	1.00	0.00	3A	
ATOM	443	С	ARG	104	20.801	-0.116	27.892	1.00	0.00	3A	
MOTA	444	0	ARG	104	21.996	~0.173	28.177	1.00	0.00	3A	
MOTA	445	N	ARG	105	19.899	-0.953	28.439	1.00	0.00	3A 3A	
ATOM	446	CA	ARG ARG	105 105	20.180 18.917	-1.924 -2.306	29.470 30.269	1.00	0.00	3A	
ATOM ATOM	447 448	CB CG	ARG	105	18.288	-1.109	31.012	1.00	0.00	3A	
ATOM	449	CD	ARG	105	17.273	-0.267	30.201	1.00	0.00	3A	
ATOM	450	NE	ARG	105	16.999	1.019	30.940	1.00	0.00	3A	
ATOM	451	CZ	ARG	105	17.736	2.168	30.769	1.00	0.00	3A 3A	
ATOM	452		ARG	105	17.471 18.734	3.253 2.262	31.550 29.841	1.00	0.00	3 <i>P</i>	
ATOM ATOM	453 454	NH2	ARG ARG	105 105	20.851	-3.183	28.984	1.00	0.00	37	
ATOM	455	o	ARG	105	21.862	-3.545	29.576	1.00	0.00	37	۹4
ATOM	456	N	PRO	106	20.439	-3.879	27.908	1.00	0.00	37	
ATOM	457	CA	PRO	106	21.118	-5.066	27.409	1.00	0.00	37	
ATOM	458	CD	PRO	106	19.166	-3.707	27.212	1.00	0.00		A 4 A 4
ATOM	459	CB	PRO	106 106	20.292 19.354	-5.535 -4.383	26.208 25.861	1.00	0.00		N 4
ATOM ATOM	460 461	CG	PRO PRO	106	22.531	-4.785	26.960	1.00	0.00		A 4
- 1 A VII		~									

ATOM	462	0	PRO	106	23.412	-5.580	27.239	1.00	0.00	3A4
MOTA	463	N ·	PHE	107	22.789	-3.612	26.347	1.00	0.00	3A4
MOTA	464	CA	PHE	107	24.092	-3.149	25.939	1.00	0.00	3A4
ATOM	465	CB	PHE	107	23.996	-1.854	25.067	1.00	0.00	3A4 3A4
ATOM	466	CG	PHE	107 107	23.377 - 24.194	-2.185	23.730 22.604	1.00	0.00	- 3A4
ATOM ATOM	467 468		PHE	107	21.982	-2.301	23.578	1.00	0.00	3A4
ATOM	469		PHE	107	23.633	-2.730	21.360	1.00	0.00	3A4
ATOM	470		PHE	107	21.415	-2.640	22.342	1.00	0.00	3A4
ATOM	471	CZ	PHE	107	22.243	-2.850	21.231	1.00	0.00	3A4
ATOM	472	С	PHE	107	24.996	-2.874	27.117	1.00	0.00	3A4
ATOM	473	0	PHE	107	26.183	-3.178	27.071	1.00	0.00	3A4
ATOM	474	N	GLY	108 108	24.445 25.169	-2.352 -2.115	28.235 29.465	1.00	0.00	3A4 3A4
ATOM ATOM	475 476	CA C	GLY	108	25.703	-3.372	30.122	1.00	0.00	3A4
ATOM	477	ŏ	GLY	108	26.825	-3.365	30.623	1.00	0.00	3A4
ATOM	478	N .	PRO	109	24.957	-4.476	30.112	1.00	0.00	3A4
ATOM	479	CA	PRO	109	25.476	-5.825	30.348	1.00	0.00	3A4
ATOM	480	CD	PRO	109	24.065	-4.305	31.286	1.00	0.00	3A4
ATOM	481	CB	PRO	109	24.191	-6.637	30.615	1.00	0.00	3A4
ATOM	482	CG	PRO	109	23.330 26.330	-5.658 -6.541	31.433 29.318	1.00	0.00	3A4 3A4
ATOM	483 484	C O	PRO PRO	109 109	27.456	-6.908	29.658	1.00	0.00	3A4
ATOM	485	N	VAL	110	25.774	-6.864	28.119	1.00	0.00	3A4
ATOM	486	CA	VAL	110	26.331	-7.778	27.133	1.00	0.00	3A4
ATOM	487	CB	VAL	110	25.389	-8.936	26.768		0.00	3A4
ATOM	488		VAL	110	25.412	-9.943	27.938	1.00	0.00	3A4
ATOM	489		VAL	110	23.943	-8.492	26.450	1.00	0.00	3A4
ATOM	490	C	VAL	110 110	26.744 25.981	-6.971 -6.165	25.923 25.392	1.00	0.00	3A4 3A4
ATOM ATOM	491 492	И	VAL GLY	111	28.021	-7.174	25.497	1.00	0.00	3A4
ATOM	493	CA	GLY	111	28.732	-6.403	24.496	1.00	0.00	3A4
ATOM	494	C	GLY	111	29.773	-5.622	25.245	1.00	0.00	3A4
ATOM	495	0	GLY	111	29.468	-4.588	25.839	1.00	0.00	3A4
ATOM	496	N	PHE	112	31.035	-6.136	25.266	1.00	0.00	3A4 3A4
ATOM	497 498	CA CB	PHE	112 112	32.105 32.907	-5.711 -6.929	26.158 26.720	1.00	0.00	3A4
ATOM ATOM	499	CG	PHE	112	31.979	-7.800	27.529	1.00	0.00	3A4
ATOM	500		PHE	112	31.631	-9.095	27.096	1.00	0.00	3A4
ATOM	501	CD2	PHE	112	31.424	-7.318	28.732	1.00	0.00	3A4
MOTA	502		PHE	112	30.746	-9.883	27.847	1.00	0.00	3A4
MOTA	503		PHE	112	30.537	-8.104	29.480	1.00	0.00	3A4 3A4
ATOM	504 505	CZ C	PHE	112 112	30.195 33.050	-9.387 -4.749	29.035 25.472	1.00	0.00	3A4
ATOM ATOM	506	o	PHE	112	34.190	-5.078	25.148	1.00	0.00	3A4
ATOM	507	N	MET	113	32.562	-3.489	25.295	1.00	0.00	3A4
ATOM	508	CA	MET	113	33.296	-2.314	24.869	1,00	0.00	3A4
ATOM	509	CB	MET	113	32.602	-1.505	23.728	1.00	0.00	3A4
MOTA	510	CG	MET	113	32.554	-2.210	22.356	1.00	0.00	3A4 3A4
ATOM ATOM	511 512	SD CE	MET MET	113 113	31.429 29.851	-3.639 -2.787	22.184 22.471	1.00	0.00	3A4
ATOM	513	C	MET	113	33.386	-1.481	26.125	1.00	0.00	3A4
ATOM	514	ō	MET	113	32.371	-1.027	26.652	1.00	0.00	3A4
ATOM	515	N	LYS	114	34.630	-1.321		1.00	0.00	3A4
ATOM	516	CA	LYS	114	34.932	-0.910	28.025	1.00	0.00	3A4
ATOM	517	CB	LYS	114	36.207	-1.643	28.544	1.00	0.00	3A4 3A4
ATOM ATOM	518 519	CD	LYS LYS	114 114	36.129 37.411	-3.170 -3.890	28.392 28.832	1.00	0.00	3A4
ATOM	520	CE	LYS	114	37.355	-5.417	28.667	1.00	0.00	3A4
ATOM	521	NZ	LYS	114	37.190	-5.806	27.244	1.00	0.00	3A4
ATOM	522	С	LYS	114	35.074	0.600	28.136	1.00	0.00	3A4
ATOM	523	0	LYS	114	34.485	1.339	27.348	1.00	0.00	3A4
ATOM	524	N	SER	115	35.857	1.092	29.141	1.00	0.00	3A4 3A4
ATOM	525	CA	SER	115	35.955 36.419	2.486 2.597	29.566 31.048	1.00	0.00	3A4 3A4
MOTA MOTA	526 527	CB OG	SER SER	115 115	35.505	1.921	31.901	1.00	0.00	3A4
ATOM	528	c	SER	115	36.891	3.307	28.696	1.00	0.00	3A4
ATOM	529	ŏ	SER	115	38.106	3.302	28.890	1.00	0.00	3A4
MOTA	530	N	ALA	116	36.300	4.041	27.709	1.00	0.00	3A4
ATOM	531	CA	ALA	116	36.990	4.902	26.770	1.00	0.00	3A4
ATOM	532	СВ	ALA	116	36.806	4.440	25.323	1.00	0.00	3A4 3A4
ATOM	533	С	ALA	116	36.445	6.277	26.942	1.00	3.50	JAN

ATOM	534	0	ALA	116	35.934	6.634	27.995	1.00	0.00	3A4
ATOM	535	N	ILE	117	36.498	7.116	25.886	1.00	0.00	3A4
MOTA	536	CA	ILE	117	36.054	8.497	25.985	1.00	0.00	3A4 3A4
ATOM	537	CB	ILE	117	36.818	9.363	24.999	1.00	0.00	3A4 3A4
ATOM	538	CG2		117	36.637 · 36.647	8.922 10.857	23.524 25.212	1.00	0.00	3A4
MOTA	539	CG1		117 117	37.122	11.262	26.574	1.00	0.00	3A4
ATOM	540	CD	ILE	117	34.556	8.659	25.822	1.00	0.00	3A4
MOTA	541 542	C O	ILE	117	33.924	9.474	26.492	1.00	0.00	3A4
MOTA MOTA	543	N	SER	118	33.923	7.843	24.946	1.00	0.00	3A4
ATOM	544	CA	SER	118	32.533	8.033	24.588	1.00	0.00	3A4
ATOM	545	СВ	SER	118	32.205	7.525	23.146	1.00	0.00	3A4
ATOM	546	OG :	SER	118	32.499	6.147	22.946	1.00	0.00	3A4 . 3A4
ATOM	547	С	SER	. 118	31.585	7.455	25.606 25.524	1.00	0.00	3A4
ATOM	548	0	SER	118	30.395	7.686 6.735	26.630	1.00	0.00	3A4
ATOM	549	N	ILE	119	32.084 31.251	6.157	27.657	1.00	0.00	3A4
ATOM	550	CA	ILE	119 119	31.480	4.637	27.705	1.00	0.00	3A4
ATOM	551 552	CB	ILE	119	32.895	4.296	28.225	1.00	0.00	3A4
ATOM ATOM	553		ILE	119	30.373	3.794	28.400	1.00	0.00	3A4
ATOM	554	CD	ILE	119	29.071	3.681	27.605	1.00	0.00	3A4
ATOM	555	c	ILE	119	31.475	6.827	29.005	1.00	0.00	3A4
ATOM	556	0	ILE	119	30.894	6.426	30.013	1.00	0.00	3A4 3A4
MOTA	557	N	ALA	120	32.350	7.862	29.050	1.00	0.00 0.00	3A4
MOTA	558	CA	ALA	120	32.876	8.420 8.417	30.276 30.275	1.00	0.00	3A4
MOTA	559	СВ	ALA	120	34.429 32.403	9.821	30.537	1.00	0.00	3A4
MOTA	560	С 0	ALA ALA	120 120	32.153	10.624	29.642	1.00	0.00	3A4
ATOM ATOM	561 562	N	GLU	121	32.338	10.132	31.847	1.00	0.00	3A4
MOTA	563	CA	GLU	121	31.987	11.402	32.421	1.00	0.00	3A4
ATOM	564	СВ	GLU	121	31.189	11.213	33.742	1.00	0.00	3A4
ATOM	565	CG	GLU	121	29.884	10.420	33.613	1.00	0.00	3A4 3A4
MOTA	566	CD	GLU	121	30.124	8.902	33.618	1.00	0.00 0.00	3A4
MOTA	567		GLU	121	29.800	8.241 8.385	32.594 34.649	1.00	0.00	3A4
MOTA	568		GLU	121 121	30.631 33.282	12.104	32.738	1.00	0.00	3A4
ATOM	569	С 0	GLU	121	34.307	11.460	32.947	1.00	0.00	3A4
MOTA MOTA	570 571	N	ASP	122	33.267	13.450	32.868	1.00	0.00	3A4
ATOM	572	CA	ASP	122	34.366	14.255	33.384	1.00	0.00	3A4
ATOM	573	СВ	ASP	122	33.940	15.762	33.320	1.00	0.00	3A4
ATOM	,574	CG	ASP	122	35.057	16.786	33.606	1.00	0.00	3A4 3A4
MOTA	575		ASP	122	34.911	17.556	34.593	1.00	0.00	3A4
MOTA	576		ASP	122	36.057 34.615	16.817	32.842 34.870	1.00	0.00	3A4
ATOM	577.	C	ASP	122 122	33.636	13.610	35.566	1.00	0.00	3A4
ATOM	578 579	O N	ASP GLU	123	35.863	13.792	35.421	1.00	0.00	3A4
ATOM ATOM	580	CA	GLU	123	37.162		34.972	1.00	0.00	3A4
ATOM	581	CB	GLU	123	37.993	14.687	36.197	1.00	0.00	3A4
ATOM	582	CG	GLU	123	37.348	15.854	36.968		0.00	3A4 3A4
MOTA	583	CD	GLU	123	38.253	16.265	38.134	1.00	0.00	3A4
ATOM	584		GLU	123	38.764	17.417	38.116 39.060	1.00	0.00	3A4
MOTA	585		GLU	123	38.443 37.950	15.431 13.205	34.211	1.00	0.00	3A4
MOTA	586	C	GLU	123 123	39.000	13.494	33.638		0.00	3A4
MOTA MOTA	587 588	O N	GLU	124	37.449	11.951	34.149		0.00	3A4
ATOM	589	CA	GLU	124	38.063	10.827	33.460		0.00	3A4
ATOM	590	СВ	GLU	124	37.284	9.523	33.756			3A4
MOTA	591	CG	GLU	124	37.186	9.213	35.261			3A4 3A4
MOTA	592	CD	GLU	124	36.410	7.908	35.465			3A4
MOTA	593		GLU	124	37.010 35.204	6.933 7.870	35.993 35.096			3A4
MOTA	594		2 GLU		38.109	11.000				3A4
ATOM	595 596	C	GLU		39.087	10.727	31.279			3A4
ATOM ATOM	596 597	N	TRP		37.027	11.579			0.00	3A4
ATOM	598	CA	TRP		36.896	11.901	30.029			3A4
ATOM	599	СВ	TRP		35.456	12.317				3A4
ATOM	600	CG	TRP	125	35.096	13.136				3A4 3A4
MOTA	601		2 TRP		34.736	14.501				3A4
ATOM	602		1 TRP		34.423	12.765 13.815				3A4
ATOM	603		1 TRP		33.701 33.805	14.860				3A4
MOTA	604		2 TRP 3 TRP		35.040	15.361				3A4
MOTA	605		- 1 KE		55.576					

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ATOM	606	CZ2	TRP	125	33.124	16.059	27.921	1.00	0.00	3A4
ATOM	607	CZ3		125	34.396	16.599	29.921	1.00	0.00	3A4
ATOM	608	CH2		125	33.421	16.924	28.984 29.585	1.00	0.00	3A4 3A4
MOTA	609 610	С 0	TRP TRP	125 125	37.893 38.564	12.940 12.734	28.590	1.00	0.00	3A4
ATOM ATOM	611	N	LYS	126	38.066	14.068	30.315	1.00	0.00	3A4
ATOM	612	CA	LYS	126	38.948	15.161	29.915	1.00	0.00	3A4
ATOM	613	СВ	LYS	126	38.776	16.362	30.855	1.00	0.00	3A4
ATOM	614	CG	LYS	126	39.424	17.682	30.406	1.00	0.00	3A4
ATOM	615	CD	LYS	126	39.026 39.634	18.858 20.191	31.300 30.845	1.00 1.00	0.00	3A4 3A4
ATOM ATOM	616 617	CE NZ	LYS LYS	126 126	39.206	21.296	31.735	1.00	0.00	. 3A4
ATOM	618	c	LYS	126	40.413	14.775	29.867	1.00	0.00	3A4
ATOM	619	0	LYS	126	41.152	15.173	28.977	1.00	0.00	3A4
ATOM	620	N	ARG	127	40.830	13.884	30.785	1.00	000	3A4
ATOM	621	CA	ARG	127	42.152	13.315	30.821 32.148	1.00 1.00	0.00	3A4 3A4
ATOM ATOM	622 623	CB CG	ARG ARG	127 127	42.369 42.319	12.556 13.460	33.385	1.00	0.00	3A4
ATOM	624	CD	ARG	127	42.230	12.652	34.686	1.00	0.00	3A4
ATOM	625	NE	ARG	127	42.079	13.613	35.835	1.00	0.00	3A4
MOTA	626	CZ	ARG	127	41.521	13.267	37.040	1.00	0.00	3A4
ATOM	627		ARG	127	41.438	14.206	38.026	1.00	0.00	3A4 3A4
ATOM	628 629	NH2	ARG	127 127	41.040 42.448	12.009 12.378	37.276 29.678	1.00	0.00	3A4
ATOM ATOM	630	ŏ	ARG	127	43.503	12.464	29.060	1.00	0.00	3A4
ATOM	631	N	LEU	128	41.487	11.489	29.329	1.00	0.00	3A4
ATOM	632	CA	LEU	128	41.614	10.553	28.227	1.00	0.00	3A4
ATOM	633	CB	LEU	128	40.552	9.436	28.305	1.00	0.00	3A4 3A4
ATOM	634 635	CG	LEU	128 128	40.710 39.492	8.475 7.536	29.510 29.620	1.00	0.00	3A4
ATOM ATOM	636		LEU	128	42.026	7.670	29.503	1.00	0.00	3A4
ATOM	637	c	LEU	128	41.513	11.260	26.900	1.00	0.00	3A4
ATOM	638	0	LEU	128	42.307	10.998	26.016	1.00	0.00	3A4
ATOM	639	N	λRG	129	40.613	12.256	26.764	1.00	0.00	3A4 3A4
ATOM	640 641	CA CB	ARG ARG	129 129	40.455 39.248	13.056 13.995	25.570 25.706	1.00	0.00	3A4
ATOM ATOM	642	CG	ARG	129	38.865	14.698	24.411	1.00	0.00	3A4
ATOM	643	CD	ARG	129	37.443	15.285	24.477	1.00	0.00	3A4
MOTA	644	NE	ARG	129	36.965	15.632	23.089	1.00	0.00	3A4
MOTA	645	CZ	ARG	129	37.094	16.870	22.512	1.00 1.00	0.00	3A4 3A4
ATOM	646 647		ARG	129 129	36.589 37.709	17.069 17.907	21.260 23.155	1.00	0.00	3A4
ATOM ATOM	648	C	ARG	129	41.673	13.896	25.247	1.00	0.00	3A4
ATOM	649	0	ARG	129	. 42.125	13.963	24.109	1.00	0.00	3A4
ATOM	650	N	SER	130	42.292	14.491	26.294	1.00	0.00	3A4
MOTA	651	CA	SER	130	43.486 43.870	15.299 16.030	26.191 27.515	1.00	0.00	3A4 3A4
MOTA MOTA	652 653	CB OG	SER	130 130	42.925	17.049	27.812	1.00	0.00	3A4
ATOM	654	c	ŞER	130	44.691	14.547	25.703	1.00	0.00	3A4
ATOM	655	0	SER	130	45.506	15.121		1.00	0.00	3A4
ATOM	656	N	LEU	131	44.822	13.241	26.004	1.00	0.00	3A4 3A4
ATOM	657 658	CA CB	LEU	131 131	45.894 45.835	12.396 11.013	25.508 26.195	1.00	0.00	3A4
MOTA MOTA	659		LEU	131	46.473	11.008	27.591		0.00	3A4
ATOM	660		LEU	131	45.836	9.924	28.474	1.00	0.00	3A4
ATOM	661	CD2	LEU	131	48.005	10.845	27.482		0.00	3A4
ATOM	662	c	LEU	131	45.875	12.189	24.006 23.361	1.00	0.00	3A4 3A4
MOTA MOTA	663 664	о и	LEU	131 132	46.913 44.675	12.177 12.059	23.421	1.00	0.00	3A4
ATOM	665	CA	LEU	132	44.436	11.692	22.040	1.00	0.00	3A4
MOTA	666	СВ	LEU	132	43.113	10.883	21.884	1.00	0.00	3A4
ATOM	667	CG	LEU	132	42.628	10.220	23.187	1.00	0.00	3A4 3A4
ATOM	668		LEU	132 132	41.170 43.579	9.739 9.147	23.225 23.759	1.00	0.00	3A4
ATOM ATOM	669 670	CDZ	LEU	132	44.339	12.896	21.142	1.00	0.00	3A4
ATOM	671	ō	LEU	132	44.709	12.862	19.975	1.00	0.00	3A4
ATOM	672	N	SER		43.808	14.009	21.685	1.00	0.00	3A4
MOTA	673	CA	SER		43.570	15.239	20.967	1.00	0.00	3A4 3A4
MOTA	674	CB OG	SER		42.882 43.525	16.277 16.664	21.854 23.058	1.00	0.00	3A4
ATOM ATOM	675 676	C	SER		44.766	15.878	20.280	1.00	0.00	3A4
ATOM	677	ŏ	SER		44.586	16.429	19.192	1.00	0.00	3A4

ATOM	678	N	PRO	134	46.017	15.798	20.777	1.00	0.00	3A4
ATOM	679	CA	PRO	134	47.159	16.327	20.076	1.00	0.00	3A4
MOTA	680	CD	PRO	134	46.405	15.537	22.155	1.00	0.00	3A4
ATOM	681	СВ	PRO	134	48.327	16.318 16.387	21.087 22.434	1.00	0.00	3A4 3A4
MOTA	682 683	CG C	PRO PRO	134 134	47.635 47.567	15.563	18.844	1.00	0.00	3A4
ATOM ATOM	684	ō	PRO	134	48.106	16.175	17.927	1.00	0.00	3A4
ATOM	685	N	THR	135	47.305	14.235	18.803	1.00	0.00	3A4
ATOM	686	CA	THR	135	47.657	13.342	17.727	1.00	0.00	3A4
ATOM	687	СВ	THR	135	47.864	11.912	18.232	1.00	0.00	3A4 3A4
ATOM	688	OG1		135 135	46.681 48.889	11.299 11.953	18.729 19.387	1.00	0.00	3A4
ATOM ATOM	689 690	CG2 C	THR	135	46.639	13.419	16.594	1.00	0.00	3A4
ATOM	691	ŏ	THR	135	46.921	13.057	15.460	1.00	0.00	3A4
ATOM	692	N	PHE	136	45.420	13.916	16.895	1.00	0.00	3A4
MOTA	693	CA	PHE	136	44.322	13.979	15.962	1.00	0.00	3A4
ATOM	694	CB	PHE	136	43.007 43.069	13.434 12.028	16.581 17.109	1.00	0.00	3A4 3A4
ATOM ATOM	695 696	CG CD1	PHE	136 136	42.397	11.733	18.297	1.00	0.00	3A4
ATOM	697	CD2		136	43.793	10.992	16.495	1.00	0.00	3A4
ATOM	698		PHE	136	42.237	10.417	18.717	1.00	0.00	3A4
ATOM	699		PHE	136	43.668	9.665	16.926	1.00	0.00	3A4
MOTA	700	CZ	PHE	136	42.847	9.372	18.017	1.00	0.00	3A4 3A4
ATOM	701 702	С 0	PHE	136 136	44.074 42.971	15.402 15.703	15.465 15.025	1.00	0.00	3A4
ATOM ATOM	703	N	THR	137	45.088	16.323	15.493	1.00	0.00	3A4
MOTA	704	CA	THR	137	44.944	17.764	15.224	1.00	0.00	3A4
MOTA	705	CB	THR	137	46.098	18.572	15.830	1.00	0.00	3A4
ATOM	706		THR	137	46.156	18.321	17.228	1.00	0.00	3A4 3A4
ATOM	707		THR	137	45.936 44.796	20.108 18.094	15.640 13.739	1.00	0.00	. 3A4
ATOM ATOM	708 709	С О	THR THR	137 137	43.885	18.830	13.359	1.00	0.00	3A4
ATOM	710	N	SER	138	45.685	17.534	12.870	1.00	0.00	3A4
ATOM	711	CA	SER	138	45.656	17.677	11.419	1.00	0.00	3A4
MOTA	712	CB	SER	138	47.076	17.874	10.806	1.00	0.00	3A4 3A4
ATOM	.713	OG	SER	138	47.648 45.012	19.086 16.431	11.280 10.860	1.00	0.00	3A4
ATOM ATOM	714 715	С 0	SER SER	138 138	43.868	16.450	10.408	1.00	0.00	3A4
ATOM	716	N	GLY	139	45.756	15.304	10.953	1.00	0.00	3A4
ATOM	717	CA	GLY	139	45.288	13.957	10.734	1.00	0.00	3A4
MOTA	718	С	GLY	139	45.698	13.207	11.960	1.00	0.00	3A4 3A4
ATOM	719	0	GLY	139 140	46.061 45.629	13.818 11.847	12.961 11.918	1.00	0.00	3A4
ATOM ATOM	720 721	N CA	LYS LYS	140	45.777	10.945	13.054	1.00	0.00	3A4
ATOM	722	СВ	LYS	140	44.729	9.786	13.048	1.00	0.00	· 3A4
ATOM	723	CG	LYS	140	43.246	10.097	13.336	1.00	0.00	3A4
MOTA	724	CD	LYS	140	42.846	11.560	13.252 13.770	1.00	0.00	3A4 3A4
ATOM	725 726	CE NZ	LYS LYS	140 140	41.456 41.193	11.872	13.770	1.00	0.00	3A4
ATOM ATOM	727	C	LYS	140	47.165	10.340	13.065	1.00	0.00	3A4
ATOM	728	ō	LYS	140	47.330	9.123	12.976	1.00	0.00	3A4
MOTA	729	N	LEU	141	48.195	11.212	13.185	1.00	0.00	3A4
ATOM	730	CA	LEU	141	49.585	10.835 10.321	13.207 11.825	1.00	0.00	3A4 3A4
ATOM ATOM	731 732	CB CG	LEU	141 141	50.096 51.411	9.530	11.812	1.00	0.00	3A4
ATOM	733		LEU	141	52.059	9.603	10.425	1.00	0.00	3A4
ATOM	734	CD2	LEU	141	51.161	8.066	12.211	1.00	0.00	3A4
ATOM	735	С	LEU	141	50.286	12.100	13.623	1.00	0.00	3A4 3A4
ATOM	736	0	LEU	141	50.455 50.687	12.362 12.924	14.813 12.618	1.00	0.00	3A4
ATOM ATOM	737 738	N CA	LYS	142 142	51.307	14.222	12.760	1.00	0.00	3A4
ATOM	739	СВ	LYS	142	52.868	14.192	12.729	1.00	0.00	3A4
ATOM	740	CG	LYS	142	53.516	13.465	13.915	1.00	0.00	3A4
ATOM	741	CD	LYS	142	55.045	13.555	13.916	1.00	0.00	3A4 3A4
ATOM	742	CE	LYS	142	55.714 55.454	12.858 11.401	15.108 15.086	1.00	0.00	3A4 3A4
ATOM ATOM	743 744	NZ C	LYS LYS	142 142	50.813	15.068	11.606	1.00	0.00	3A4
ATOM	745	ŏ	LYS	142	50.704	16.287	11.736	1.00	0.00	3A4
MOTA	746	N	GLU	143	50.529	14.432	10.433	1.00	0.00	3A4
MOTA	747	CA	GLU	143	50.169	15.105	9.198 8.234	1.00	0.00	3A4 3A4
ATOM ATOM	748 749	CB CG	GLU	143 143	51.389 51.158	15.242 16.046	6.935	1.00	0.00	3A4
ALUM	143	~ ~	2110	A 3 -						

ATOM	750	CD	GLU	143	50.774	17.493	7.267	1.00	0.00	3A4
ATOM	751	OE1		143	51.602	18.194	7.909		0.00	3A4
ATOM	752	OE2		143	49.651	17.917	6.882		0.00	3A4
ATOM	753	С	GLU	143	49.047	14.324	8.559	_	0.00	3A4 3A4
ATOM	754	0	GLU	143	47.898	14.760	8.605	1.00	0.00	3A4
MOTA	755	N	MET	144	49.393	13.160	7.926 7.300	1.00	0.00	3A4
MOTA	756	CA	MET	144	48.584	12.130 11.759	8.070	1.00	0.00	3A4
ATOM	757	СВ	MET	144	47.303 47.567	10.932	9.334	1.00	0.00	3A4
MOTA	758 759	CG SD	MET MET	144 144	48.269	9.267	9.019	1.00	0.00	3A4
ATOM ATOM	760	CE	MET	144	47.029	8.504	7.928	1.00	0.00	3A4
ATOM	761	c	MET	144	48.192	12.409	5.879	1.00	0.00	3A4
ATOM	762	ō	MET	144	47.891	11.472	5.150	1.00	0.00	3A4
ATOM	763	N	VAL	145	48.169	13.678	5.428	1.00	0.00	3A4 3A4
ATOM	764	CA	VAL	145	47.650	14.088	4.130 3.949	1.00	0.00	3A4
MOTA	765	СВ	VAL	145	47.693	15.597	2.734	1.00	0.00	3A4
ATOM	766		VAL	145	46.839 47.128	16.061 16.245	5.237	1.00	0.00	3A4
ATOM	767	C	VAL VAL	145 145	48.261	13.425	2.906	1.00	0.00	3A4
ATOM ATOM	768 769	ō	VAL	145	47.501	13.014	2.026	1.00	0.00	3A4
ATOM	770	N	PRO	146	49.595	13.235	2.821	1.00	0.00	3A4
ATOM	771	CA	PRO	146	50.226	12.490	1.741	1.00	0.00	3A4
ATOM	772	CD	PRO	146	50.623	13.942	3.599	1.00	0.00	3A4
ATOM	773	CB	PRO	146	51.743	12.625	1.988	1.00	0.00	3A4 3A4
ATOM	774	CG	PRO	146	51.872	13.954	2.721	1.00	0.00	3A4
MOTA	775	С	PRO	146	49.826	11.029 10.483	1.698 0.613	1.00	0.00	3A4
ATOM	776	0	PRO	146 147	49.678 49.572	10.483	2.863	1.00	0.00	3A4
ATOM	777 778	N CA	ILE	147	49.098	9.027	2.976	1.00	0.00	3A4
ATOM ATOM	779	СВ	ILE	147	49.254	8.469	4.382	1.00	0.00	3A4
ATOM	780		ILE	147	48.993	6.930	4.422	1.00	0.00	3A4
ATOM	781		ILE	147	50.685	8.809	4.901	1.00	0.00	3A4
MOTA	782	CD	ILE	147	51.018	8.281	6.300	1.00	0.00	3A4 3A4
ATOM	783	С	ILE	147	47.660	8.881	2.564	1.00	0.00 0.00	3A4
ATOM	784	0	ILE	147	47.306	7.899 9.866	1.922 2.875	1.00	0.00	3A4
MOTA	785	N	ILE	148 148	46.789 45.386	9.833	2.503	1.00	0.00	3A4
MOTA	786 787	CA CB	ILE	148	44.570	10.932	3.172	1.00	0.00	3A4.
MOTA MOTA	788		ILE	148	43.057	10.768	2.811	1.00	0.00	3A4
ATOM	789		ILE	148	44.675	10.809	4.718	1.00	0.00	3A4
ATOM	790	CD	ILE	148	44.158	12.030	5.488	1.00	0.00	3A4
MOTA	791	С	ILE	148	45.218	9.888	1.005		0.00	3A4 3A4
MOTA	792	0	ILE	148	44.486	9.106	0.407 0.350	1.00	0.00	3A4
MOTA	793	N	ALA	149	46.000 46.058	10.765 10.923	-1.086	1.00	0.00	3A4
MOTA	794	CA	ALA ALA	149 149	46.983	12.097	-1.414	1.00	0.00	3A4
ATOM ATOM	795 796	CB C	ALA	149	46.539	9.682	-1.803	1.00	0.00	3A4
ATOM	797	ō	ALA	149	45.965	9.246	-2.797	1.00	0.00	/ 3A4
ATOM	798	N	GLN	150	47.578	9.019	-1.243	1.00	.0.00	3A4
ATOM	799	CA	GLN	150	48.121	7.780	-1.753	1.00	0.00	3A4 3A4
MOTA	800	СВ	GLN	150	49.342	7.295	-0.954	1.00	0.00	3A4
MOTA	801	CG	GLN	150	50.637	8.037 7.586	-1.297 -0.326	1.00	0.00	3A4
MOTA	802	CD	GLN	150	51.737 52.080		-0.292		0.00	3A4
ATOM	803 804		GLN	150 150	52.300	8.525	0.483	1.00	0.00	3A4
ATOM ATOM	805	C	GLN	150	47.129	6.663	-1.774	1.00	-0.00	3A4
ATOM	806	ō	GLN		46.962	5.992	-2.789		0.00	3A4
ATOM	807	N	TYR	151	46.371	6.500	-0.658	1.00	0.00	3A4 3A4
ATOM	808	CA	TYR		45.418	5.431	-0.538		0.00	3A4
MOTA	809	CB	TYR		44.853	5.227	0.859 0.880			3A4
MOTA	810	CG	TYR		44.181 43.188	3.823 3.417	1.745			3A4
MOTA	811 812		TYR TYR		44.795	2.750	0.124			3A4
ATOM ATOM	813		TYR		42.443	2.274	1.345	1.00	0.00	3A4
ATOM	814		TYR		44.170	1.533	-0.113	1.00		3A4
ATOM	815	CZ	TYR		42.935	1.315	0.454			3A4
ATOM	816	OH	TYR		42.254	0.104	0.201			3A4
MOTA	817	С	TYR		44.221	5.669	-1.449			3A4 3A4
ATOM	818	0	TYR		43.738		-2.103			3A4
MOTA	819	N	GLY		43.775		-1.554 -2.423			3A4
MOTA	820	CA	GLY		42.703 42.962		-3.877			3A4
MOTA	821	С	GLY	174	42.502			-		

ATOM	822	0	GLY	152	42.122	6.466	-4.565	1.00	0.00	3A4
ATOM	823	N	ASP	153	44.194	7.284	-4.339	1.00	0.00	3A4
ATOM	824	CA	ASP	153	44.647	6.996	-5.674	1.00	0.00	3A4
	825			153	46.061	7.586	-5.844	1.00	0.00	3A4
MOTA		CB	ASP		45.993	9.119	-5.945	1.00	0.00	3A4
ATOM	826	CG	ASP	153			-6.534	1.00	0.00	3A4
ATOM	827	OD1		153	45.014	9.650		1.00	0.00	3A4
MOTA	828	OD2		153	46.922	9.784	-5.416		0.00	3A4
MOTA	829	С	ASP	153	44.703	5.521	-6.007	1.00	0.00	3A4
MOTA	830	0	ASP	153	44.288	5.096	-7.076	1.00		3A4
ATOM	831	N	VAL	154	45.154	4.686	-5.048	1.00	0.00	
ATOM	832	CA	VAL	154	45.173	3.235	-5.160	1.00	0.00	3A4
ATOM	833	CB	VAL	154	45.878	2.605	-3.968	1.00	0.00	3A4
ATOM	834	CG1	VAL	154	45.770	1.054	-3.875	1.00	0.00	3A4
ATOM	835	CG2	VAL	154	47.373	2.989	-4.067	1.00	0.00	3A4
ATOM	836	С	VAL	154	43.793	2.651	-5.283	1.00	0.00	3A4
ATOM	837	0	VAL	154	43.531	1.783	-6.112	1.00	0.00	3A4
ATOM	838	N	LEU	155	42.842	3.184	-4.494	1.00	0.00	3A4
ATOM	839	CA	LEU	155	41.460	2.758	-4.505	1.00	0.00	3A4
ATOM	840	СB	LEU	155	40.697	3.480	-3.395	1.00	0.00	3A4
ATOM	841	CG	LEU	155	41.005	3.018	-1.989	1.00	0.00	3A4
	842		LEU	155	40.785	4.226	-1.096	1.00	0.00	3A4
ATOM				155	40.117	1.825	-1.591	1.00	0.00	3A4
MOTA	843		LEU		40.732	3.082	-5.782	1.00	0.00	3A4
ATOM	844	C	LEU	155		2.295	-6.313	1.00	0.00	3A4
ATOM	845	0	LEU	155	39.955			1.00	0.00	3A4
ATOM	846	N	VAL	156	41.020	4.276	-6.333	1.00	0.00	3A4
MOTA	847	CA	VAL	156	40.441	4.744	-7.564			3A4
ATOM .	848	CB	VAL	156	40.709	6.216	-7.769	1.00	0.00	3A4
MOTA	849		VAL	156	40.208	6.709	-9.147	1.00		· 3A4
MOTA	850	CG2	VAL	156	39.887	6.989	-6.709	1.00	0.00	
MOTA	851	С	VAL	156	40.956	3.916	-8.726	1.00	0.00	3A4
MOTA	852	0	VAL	156	40.186	3.474	-9.566	1.00	0.00	3A4
ATOM	853	N	ARG	157	42.263	3.571	-8.714	1.00	0.00	3A4
ATOM	854	CA	ARG	157	42.881	2.692	-9.687	1.00	0.00	3A4
MOTA	855	СВ	ARG	157	44.400	2.603	-9.480	1.00	0.00	3A4
ATOM	856	CG	ARG	157	45.201	1.988	-10.646	1.00	0.00	3A4
ATOM	857	CD	ARG	157	46.718	1.949	-10.406	1.00	0.00	3A4
ATOM	858	NE	ARG	157	47.008	0.982	-9.282	1.00	0.00	3A4
ATOM	859	CZ	ARG	157	47.582	1.328	-8.084	1.00	0.00	3A4
ATOM	860		ARG	157	47.753	0.362	-7.136	1.00	0.00	3A4
ATOM	861		ARG	157	47.975	2.607	-7.807	1.00	0.00	3A4
ATOM	862	c	ARG	157	42.316	1.305	-9.694	1.00	0.00	. 3A4
ATOM	863	õ.	ARG	157	42.062		-10.749	1.00	0.00	3A4
	864	N	ASN	158	42.004	0.746	-8.509	1.00	0.00	3A4
ATOM		CA	ASN	158	41.363	-0.540	-8.359	1.00	0.00	3A4
ATOM	865		ASN	158	41.312	-0.962	-6.875	1.00	0.00	3A4
MOTA	866	CB			42.725	-1.184	-6.308	1.00	0.00	3A4
ATOM	867	CG	ASN	158	43.710	-1.336	-7.029	1.00	0.00	3A4
ATOM	868		ASN	158		-1.211	-4.951	1.00	0.00	3A4
ATOM	869		ASN	158	42.827 39.959	-0.569	-8.928		0.00	3A4
ATOM	870	C	ASN	158				1.00	0.00	3A4
ATOM	871	0	ASN	158	39.541	-1.568	-9.503 -8.840		0.00	. 3A4
ATOM	872	N	LEU	159	39.205	0.547		1.00	0.00	3A4
ATOM	873	CA	LEU	159	37.900	0.698	-9.460			3A4
ATOM	874	СB	LEU	159	37.181	1.944	-8.901	1.00	0.00	3A4
ATOM	875	CG	LEU	159	36.392	1.845			0.00	
ATOM	876	CD1	LEU	159	35.846	3.252	-7.275	1.00	0.00	3A4
ATOM	877	CD2	LEU	159	35.226	0.844	-7.672	1.00	0.00	3A4
ATOM	878	С	LEU	159	37.986		-10.979	1.00	0.00	3A4
ATOM	879	0	LEU	159	37.180		-11.731	1.00	0.00	3A4
ATOM	880	N	ARG	160	39.032		-11.475	1.00	0.00	3A4
ATOM	881	CA	ARG	160	39.316		-12.887	1.00	0.00	3A4
ATOM	882	СВ	ARG	160	40.462		-13.097	1.00	0.00	3A4
ATOM	883	ĊĠ	ARG	160	40.032		-12.829	1.00	0.00	3A4
ATOM	884	CD	ARG	160	41.097		-13.106	1.00	0.00	3A4
ATOM	885	NE	ARG	160	42.243		-12.147	1.00	0.00	3A4
ATOM	886	CZ	ARG	160	43.077		-11.785	1.00	0.00	3A4
	887		ARG	160	44.114		-10.932		0.00	3A4
ATOM	888		ARG	160	42.889		-12.251	1.00	0.00	3A4
ATOM				160	39.687		-13.585		0.00	3A4
ATOM	889	C	ARG		39.428		-14.767		0.00	3A4
ATOM	890	0	ARG	160			-12.834		0.00	3A4
MOTA	891	И	ARG	161	40.250		-13.293		0.00	3A4
MOTA	892	CA	ARG	161	40.597		-12.420			3A4
MOTA	893	СB	ARG	161	41.743	-2.432	-12.420	1.00	5.00	J

ATOM	894	CG	ARG	161	43.082	-1.717 -12.670	1.00	0.00	3A4
ATOM	895	CD	ARG	161	44.093	-1.838 -11.519	1.00	0.00	3A4
ATOM	896	NE	ARG	161	44.400	-3.285 -11.257	1.00	0.00	3A4 3A4
ATOM	897	CZ	ARG	161 161	45.172 45.396	-3.692 -10.198 -5.024 -10.010	1.00	0.00	3A4
ATOM	898 899	NH1 NH2		161	45.720	-2.792 -9.328	1.00	0.00	3A4
ATOM ATOM	900	C	ARG	161	39.432	-2.837 -13.270	1.00	0.00	3A4
ATOM	901	ŏ	ARG	161	39.618	-4.026 -13.474	1.00	0.00	3A4
ATOM	902	N	GLU	162	38.181	-2.341 -13.060	1.00	0.00	3A4
ATOM	903	CA	GLU	162	36.943	-3.106 -13.121	1.00 1.00	0.00	3A4 3A4
ATOM	904	CB	GLU	162 162	35.704 35.006	-2.403 -12.447 -1.245 -13.229	1.00	0.00	3A4
ATOM ATOM	905 906	CG CD	GLU	162	33.961	-0.524 -12.375	1.00	0.00	3A4
ATOM	907		GLU	162	34.331	-0.002 -11.289	1.00	0.00	3A4
ATOM	908	OE2	GLU	162	32.779	-0.469 -12.809	1.00	0.00	3A4
ATOM	909	С	GLU	162	36.578	-3.419 -14.538	1.00	0.00	3A4 3A4
ATOM	910	0	GLU	162	36.521	-2.577 -15.435 -4.746 -14.788	1.00	0.00	3A4
ATOM	911 912	N CA	ALA ALA	163 163	36.386 36.408	-5.391 -16.091	1.00	0.00	3A4
ATOM ATOM	913	CB	ALA	163	37.029	-6.809 -15.993	1.00	0.00	3A4
ATOM	914	c	ALA	163	35.037	-5.494 -16.717	1.00	0.00	3A4
ATOM	915	0	ALA	163	34.019	-5.308 -16.051	1.00	0.00	3A4
MOTA	916	N	GLU	164	35.042	-5.771 -18.059 -5.860 -19.009	1.00 1.00	0.00	3A4 3A4
ATOM	917	CA	GLU	164 164	33.935 32.661	-6.587 -18.459		0.00	3A4
ATOM ATOM	918 919	CB CG	GLU	164	31.701	-7.151 -19.531	1.00	0.00	3A4
ATOM	920	CD	GLU	164	30.505	-7.813 -18.839	1.00	0.00	3A4
ATOM	921	OE1	GLÜ	164	29.737	-7.082 - 18.156	1.00	0.00	3A4
MOTA	922		GLU	164	30.342	-9.055 -18.984	1.00	0.00	3A4 3A4
MOTA	923	C	GLU	164	33.612 32.462	-4.461 -19.520 -4.138 -19.797	1.00 1.00	0.00	3A4
ATOM ATOM	924 925	O N	GLU THR	164 165	34.671	-3.592 -19.572	1.00	0.00	3A4
ATOM	926	CA	THR	165	34.730	-2.131 -19.714	1.00	0.00	3A4
ATOM	927	СВ	THR	165	34.039	-1.480 -20.938	1.00	0.00	3A4
MOTA	928		THR	165	32.615	-1.557 -20.965	1.00	0.00	3A4 3A4
ATOM	929		THR	165	34.604	-2.115 -22.228 -1.470 -18.379	1.00 1.00	0.00	3A4
ATOM	930 931	С 0	THR THR	165 -165	34.372 35.235	-0.931 -17.690	1.00	0.00	3A4
ATOM ATOM	932	N	GLY	166	33.075	-1.547 -17.996	1.00	0.00	3A4
ATOM	933	CA	GLY	166	32.567	-1.129 -16.720		0.00	3A4
MOTA	934	С	GLY	166		-1.094 -16.877		0.00	. 3A4 3A4
ATOM	935	0 .	GLY	166	30.541 30.386	-0.151 -17.449 -2.143 -16.363		0.00	3A4
ATOM	936 937	N CA	LYS LYS	167 167	28.935	-2.211 -16.262		0.00	3A4
ATOM ATOM	. 938	CB	LYS	167		-3.202 -17.239		0.00	3A4
ATOM	939	CG	LYS	167	28.165	-2.770 -18.713		0.00	3A4
ATOM	940	CD	LYS	167	29.336	-3.252 -19.574		0.00	3A4 3A4
ATOM	941	CE	LYS	167	29.134 30.208	-2.949 -21.066 -3.554 -21.890		0.00	3A4
ATOM	942 943	NZ C	ĻYS LYS	167 167	28.582	-2.486 -14.802		0.00	3A4
ATOM ATOM	944	ō	LYS	167	27.816	-1.688 -14.271		0.00	3A4
ATOM	945	N	PRO	168	29.041	-3.521 -14.057		0.00	3A4
ATOM	946	CA	PRO	168	28.796	-3.641 -12.622		0.00	3A4 3A4
ATOM	947	CD	PRO	168	29.518 28.695	-4.787 -14.626 -5.165 -12.400		0.00	3A4
ATOM ATOM	948 949	CB CG	PRO PRO	168 168	29.625	-5.777 -13.459		0.00	3A4
ATOM	950	č	PRO	168	29.938	-3.027 -11.812	1.00	0.00	3A4
ATOM	951	0	PRO	168	31.100	-3.303 -12.110		0.00	3A4
MOTA	952	N	VAL	169	29.609	-2.275 -10.724		0.00	3A4 3A4
ATOM	953	CA	VAL	169	30.441 31.674	-2.280 -9.531 -1.381 -9.591		0.00	3A4
ATOM	954 955	CB	VAL VAL	169 169	31.356	0.130 -9.641			3A4
MOTA MOTA	956		VAL	169	32.702	-1.746 -8.502	1.00	0.00	3A4
MOTA	957	C	VAL	169	29.535	-1.926 -8.383			3A4
MOTA	958	0	VAL	169	28.623	-1.120 -8.520			3A4 3A4
ATOM	959	N	THR	170	29.805	-2.498 -7.184 -2.121 -5.93			3A4
ATOM	960	CA CB	THR THR	170 170	29.193 28.902	-3.314 -5.03			3A4
MOTA MOTA	961 962		THR	170	28.066	-4.231 -5.73			3A4
ATOM	963		THR	170	28.173	-2.877 -3.73	6 1.00		3A4
ATOM	964	С	THR	170	30.178	-1.183 -5.30			3A4
ATOM	965	0	THR	170	31.232	-1.589 -4.83	1 1.00	0.00	3A4

ATOM	966	N	LEU	171	29.854	0.126	-5.296	1.00	0.00	3A4
MOTA	967	CA	LEU	171	30.705	1.177	-4.769	1.00	0.00	3A4
ATOM	968	CB	LEU	171	30.055	2.555 3.319	-5.044 -6.282	1.00	0.00	3A4 3A4
ATOM ATOM	969 970	CG CD1	LEU	171 171	30.547 29.654	4.563	-6.453	1.00	0.00	3A4
ATOM	971	CD2		171	32.040	3.710	-6.194	1.00	0.00	3A4
ATOM	972	С	LEU	171	30.998	1.069	-3.277	1.00	0.00	3A4
ATOM	973	0	LEU	171	32.076	1.436	-2.831 -2.464	1.00	0.00	3A4 3A4
ATOM	974 975	N CA	LYS LYS	172 172	30.072 30.261	0.510 0.291	-1.041	1.00	0.00	3A4
ATOM ATOM	976	CB	LYS	172	28.920	-0.132	-0.376	1.00	0.00	3A4
ATOM	977	CG	LYS	172	28.909	-0.334	1.158	1.00	0.00	3A4
ATOM	978	CD	LYS	172	29.194	0.939	1.969	1.00	0.00 0.00	3A4 3A4
ATOM	979	CE NZ	LYS	172 172	29.078 30.110	0.766 -0.160	3.488 4.012	1.00	0.00	3A4
ATOM ATOM	980 981	C	LYS	172	31.330	-0.744	-0.748	1.00	0.00	3A4
ATOM	982	ō	LYS	172	32.274	-0.492	-0.010	1.00	0.00	3A4
ATOM	983	N	ASP	173	31.243	-1.937	-1.374	1.00	0.00	3A4 3A4
MOTA	984	CA	ASP	173 ° 173	32.134 31.447	-3.048 -4.365	-1.103 -1.539	1.00	0.00	3A4
ATOM ATOM	985 986	CB CG	ASP ASP	173	32.095	-5.634	-0.940	1.00	0.00	3A4
ATOM	987		ASP	173	32.129	-5.750	0.315	1.00	0.00	3A4
ATOM	988	OD2	ASP	173	32.559	-6.496	-1.735	1.00	0.00	3A4 3A4
ATOM	989	C	ASP	173	33.491 34.487	-2.909 -3.361	-1.760 -1.199	1.00	0.00	3A4
ATOM ATOM	990 991	O N	ASP VAL	173 174	33.571	-2.272	-2.947	1.00	0.00	- 3A4
ATOM	992	CA	VAL	174	34.804	-2.128	-3.702	1.00	0.00	3A4
ATOM	993	CB	VAL	174	34.550	-2.192	-5.209	1.00	0.00	3A4
ATOM	994		VAL	174	35.866	-2.225	-6.033 -5.482	1.00	0.00	3A4 3A4
ATOM ATOM	995 996	CG2	VAL	174 174	33.783 35.560	-3.513 -0.866	-3.321	1.00	0.00	3A4
ATOM	997	ŏ	VAL	174	36.767	-0.793	-3.522	1.00	0.00	3A4
ATOM	998	N	PHE	175	34.889	0.162	-2.748	1.00		3A4
ATOM	999	CA	PHE	175	35.513	1.457 2.458	-2.585 -3.637	1.00	0.00	3A4 3A4
ATOM	1000 1001	CB CG	PHE	175 175	34.996 35.738	3.789	-3.669	1.00	0.00	3A4
ATOM ATOM	1001		PHE	175	35.169	4.936	-3.079	1.00	0.00	3A4
ATOM	1003	CD2	PHE	175	37.019	3.896	-4.239	1.00	0.00	3A4
ATOM	1004		PHE	175	35.866	6.153	-3.047 -4.237	1.00	0.00	3A4 3A4
ATOM ATOM	1005 1006	CE2	PHE	175 175	37.703 37.136	5.120 6.244	-3.628	1.00	0.00	3A4
ATOM	1007	Ç	PHE	175	35.362	1.997	-1.219	1.00	0.00	3A4
ATOM	1008	0	PHE	175	36.347	2.184	-0.509	1.00	0.00	3A4
ATOM	1009	N	GLY	176	34.105	2.318	-0.836 0.352	1.00	0.00	. 3A4 3A4
ATOM ATOM	1010 1011	CA C	GLY GLY	176 176	33.755 34.098	3.060 2.332	1.609	1.00	0.00	3A4
ATOM	1011	o	GLY	176	34.413	2.958	2.614	1.00	0.00	3A4
ATOM	1013	N	ALA	177	34.126	0.976	1.565	1.00	0.00	3A4
ATOM .	1014	CA	ALA	177	34.485	. 0.144	2.688 2.532	1.00	0.00	. 3A4 3A4
ATOM ATOM	1015 1016	CB C	ALA ALA	177 177	33.968 35.962	-1.294 0.124	2.332	1.00	0.00	3A4
ATOM	1017	ŏ	ALA	177	36.406	0.327	4.080	1.00	0.00	3A4
ATOM	1018	N	TYR	178	36.777	-0.058		1.00	0.00	3A4
ATOM	1019	CA	TYR	178		-0.242	2.016	1.00	0.00	3A4 3A4
ATOM	1020 1021	CB CG	TYR TYR		38.721 38.656	-0.724 -2.235	0.638 0.593	1.00	0.00	3A4
MOTA MOTA	1021		TYR		37.893	-2.854	-0.416	1.00	0.00	3A4
ATOM	1023	CD2	TYR	178	39.236	-3.052	1.584	1.00	0.00	3A4
MOTA	1024		TYR		37.711	-4.243	-0.441	1.00	0.00	3A4 3A4
ATOM ATOM	1025 1026	CE2	TYR TYR		39.039 38.282	-4.442 -5.040	1.580 0.562	1.00	0.00	3A4
ATOM	1027	ОН	TYR		38.091	-6.439	0.553	1.00	0.00	3A4
ATOM	1028	С	TYR	178	38.966	1.017	2.362	1.00	0.00	3A4
ATOM	1029	0	TYR		39.918	0.985	3.127	1.00	0.00	3A4 3A4
ATOM ATOM	1030 1031	N CA	SER SER		38.545 39.171	2.180 3.471	1.822 2.018	1.00	0.00	3A4
ATOM	1031	CB	SER		38.412	4.545	1.196	1.00		3A4
ATOM	1033	ŌĞ	SER	179	39.108	5.787	1.074	1.00		3A4
MOTA	1034	C	SER		39.344	3.878	3.465	1.00		3A4 3A4
MOTA	1035	0	SER		40.445 38.263	4.039 3.919	3.966 4.233	1.00		3A4
ATOM ATOM	1036 1037	N CA	MET		38.263	4.314	5.621	1.00		3A4

ATOM	1038	СВ	MET	180	36.898	4.623	5.984	1.00	0.00	3A4
ATOM	1039	CG	MET	180	36.729	5.941	5.189	1.00	0.00	3A4
ATOM	1040	SD	MET	180	35.589	5.903	3.791	1.00	0.00	3A4
ATOM	1041	CE	MET	180	36.564	7.153	2.893	1.00	0.00	3A4
ATOM	1042	C	MET	180	38.961	3.325	6.527	1.00	0.00	3A4 3A4
ATOM	1043	0	MET	180	39.602 38.892	3.684 2.030	7.513 6.144	1.00	0.00	3A4
MOTA	1044	N	ASP	181 181	39.455	1.016	6.971	1.00	0.00	3A4
ATOM	1045 1046	CA CB	ASP ASP	181	38.927	-0.386	6.705	1.00	0.00	3A4
MOT'A MOTA	1045	CG	ASP	181	38.781	-1.148	5.400	1.00	0.00	3A4
ATOM	1048		ASP	181	39.773	-1.165	4.635	1.00	0.00	3A4
ATOM	1049		ASP	181	37.728	-1.810	5.195	1.00	0.00	3A4
ATOM	1050	C	ASP	181	40.963	0.976	6.884	1.00	0.00	3A4
ATOM	1051	0	ASP	181	41.663	0.876	7.886	1.00	0.00	3A4
ATOM	1052	N	VAL	182	41.515	1.163	5.671	1.00	0.00	3A4
ATOM	1053	CA	VAL	182	42.946	1.238	5.464	1.00	0.00	3A4
MOTA	1054	СВ	VAL	182	43.279	1.227	4.010	1.00	0.00	3A4
ATOM	1055		VAL	182	44.767	1.508	3.706	1.00	0.00	3A4 3A4
ATOM	1056		VAL	182	42.889	-0.181 2.408	3.532 6.151	1.00	0.00	3A4
ATOM	1057	C	VAL	182 182	43.593 44.676	2.298	6.708	1.00	0.00	3A4
MOTA MOTA	1058 1059	О И	VAL ILE	183	42.877	3.540	6.210	1.00	0.00	3A4
ATOM	1060	CA	ILE	183	43.341	4.740	6.855	1.00	0.00	3A4
ATOM	1061	CB	ILE	183	42.480	5.913	6.432	1.00	0.00	3A4
ATOM	1062		ILE	183	42.783	7.205	7.220	1.00	0.00	3A4
MOTA	1063		ILE	183	42.712	6.215	4.926	1.00	0.00	3A4
ATOM	1064	CD	ILE	183	44.121	6.672	4.516	1.00	0.00	. 3A4
MOTA	1065	С	ILE	183	43.365	4.589	8.352	1.00	0.00	3A4
MOTA	1066	0	ILE	183	44.321	4.972	9.017	1.00	0.00	3A4
ATOM	1067	N	THR	184	42.323	3.969	8.947	1.00	0.00	3A4 3A4
ATOM	1068	CA	THR	184 184	42.311 40.896	3.780 3.599	10.379 10.968	1.00	0.00	3A4
ATOM ATOM	1069 1070	CB	THR THR	184	40.842	3.873	12.369	1.00	0.00	3A4
ATOM	1070		THR	184	40.253	2.222	10.686	1.00	0.00	3A4
ATOM	1072	c	THR	184	43.288	2.710	10.811	1.00	0.00	3A4
ATOM	1073	ō	THR	184	43.934	2.838	11.842	1.00	0.00	3A4
ATOM	1074	N	SER	185	43.544	1.697	9.955	1.00	0.00	3A4
ATOM	1075	CA	SER	185	44.571	0.701	10.179	1.00	0.00	3A4
MOTA	1076	CB	SER	185	44.486	-0.452	9.173	1.00	0.00	3A4
ATOM	1077	OG	SER	185	43.278	-1.178	9.354	1.00	0.00	3A4 3A4
MOTA	1078	Ç	SER	185	45.975 46.793	1.270 0.962	10.157 11.011	1.00	0.00	3A4
ATOM	1079 1080	И	SER THR	185 186	46.255	2.211	9.238	1.00	0.00	3A4
ATOM ATOM	1081	CA	THR	186	47.523	2.905	9.158	1.00	0.00	
ATOM	1082	CB	THR	186	47.674	3.626	7.845	1.00	0.00	3A4
ATOM	1083		THR	186	46.613	4.495	7.478	1.00	0.00	3A4
ATOM	1084	CG2	THR	186	47.869	2.559	6.746	1.00	0.00	3A4
ATOM	1085	С	THR	186	47.770	3.895	10.256	1.00	0.00	3A4
ATOM	1086	0	THR	186	48.906	4.171	10.627	1.00	0.00	3A.4
MOTA	1087	N	SER	187	46.676	4.433	10.825	1.00	0.00	3A4 3A4
MOTA	1088	CA	SER	187	46.674	5.311	11.961 12.078	1.00	0.00	3A4
ATOM	1089 1090	CB OG	SER SER	187 187	45.260 45.037	5.983 6.742	13.262	1.00	0.00	3A4
ATOM ATOM	1091	C	SER	187	47.012		13.221		0.00	3A4
ATOM	1092	ō	SER	187.	47.753	5.052	14.047	1.00	0.00	3A4
ATOM	1093	N	PHE	188	46.490	3.324	13.352	1.00	0.00	3A4
MOTA	1094	CA	PHE	188	46.634	2.477	14.511	1.00	0.00	3A4
ATOM	1095	СВ	PHE	188	45.408	1.520	14.609	1.00	0.00	3A4
MOTA	1096	CG		. 188	44.440	2.221	15.507	1.00	0.00	3A4
MOTA	1097		PHE	188	43.828	3.428	15.112	1.00	0.00	3A4
MOTA	1098		PHE	188	44.425	1.853	16.860	1.00	0.00	3A4 3A4
ATOM	1099		PHE	188	43.309 43.917	4.298 2.727	16.068 17.815	1.00	0.00	3A4
ATOM	1100 1101	CEZ	PHE PHE	188 188	43.370	3.945	17.418	1.00	0.00	3A4
ATOM ATOM	1101	C	PHE	188	47.882	1.665	14.537	1.00	0.00	3A4
ATOM	1102	ò	PHE	188	48.386	1.332	15.605	1.00	0.00	3A4
ATOM	1104	N	GLY	189	48.414	1.335	13.350	1.00	0.00	3A4
ATOM	1105	ÇA	GLY	189	49.610	0.550	13.208	1.00	0.00	3A4
ATOM	1106	C	GLY	189	49.281	-0.923	13.101	1.00	0.00	3A4
MOTA	1107	0	GLY	189	50.025	-1.788	13.555	1.00	0.00	3A4
MOTA	1108	N	VAL	190	48.147	-1.240	12.428	1.00	0.00	3A4
MOTA	1109	CA	VAL	190	47.745	-2.576	12.011	1.00	0.00	3A4

	ATOM	1110	СВ	VAL	190	46.239	-2.768	11.929	1.00	0.00	3A4
	ATOM	1111	CG1		190	45.823	-4.253	11.759	1.00	0.00	3A4
	MOTA	1112	CG2		190	45.621	-2.217	13.235	1.00	0.00	3A4 3A4
	ATOM	1113	C	VAL	190	48.306 48.419	-2.843 -1.948	10.635 9.801	1.00	0.00	3A4
	ATOM ATOM	1114 1115	Ŋ	VAL ASN	190 191	48.675	-4.105	10.372	1.00	0.00	3A4
	ATOM	1116	CA	ASN	191	49.636	-4.477	9.377	1.00	0.00	3A4
	ATOM	1117	CB	ASN	191	49.869	-5.997	9.517	1.00	0.00	3A4
	ATOM	1118	CG	ASN	191	51.211	-6.502	8.934	1.00	0.00	3A4
	ATOM	1119	OD1		191	52.277	-6.160	9.445 7.848	1.00	0.00 0.00	3A4 3A4
	MOTA	1120	ND2	ASN	191 191	51.156 49.394	-7.322 -4.146	7.970	1.00	0.00	3A4
	ATOM ATOM	1121 1122	0	ASN	191	48.268	-4.363	7.523	1.00	0.00	3A4
	ATOM	1123	N	ILE	192	50.505	-3.532	7.398	1.00	0.00	3A4
	MOTA	1124	CA	ILE	192	50.796	-3.011	6.064	1.00	0.00	3A4
	MOTA	1125	CB	ILE	192	49.572	-3.045	5.191	1.00	0.00	3A4 3A4
	ATOM	1126	CG2		192 192	48.539 49.850	-2.012 -3.205	5.843 3.643	1.00	0.00	3A4
	ATOM ATOM	1127 1128	CG1	ILE	192	50.855	-4.296	3.249	1.00	0.00	3A4
	ATOM	1129	C	ILE	192	51.332	-1.562	6.101	1.00	0.00	3A4
	ATOM	1130	0	ILE	192	51.714	-1.049	7.152	1.00	0.00	3A4
	ATOM	1131	N	ASP	193	51.273	-0.876	4.912	1.00	0.00	3A4 3A4
	ATOM	1132	CA	ASP	193	51.280 52.500	0.551 0.950	4.649 3.755	1.00	0.00	3A4
	ATOM ATOM	1133 1134	CB CG	ASP ASP	193 193	52.747	2.473	3.713	1.00	0.00	3A4
	ATOM	1135		ASP	193	52.690	3.055	2.596	1.00	0.00	3A4
	ATOM	1136		ASP	193	52.993	3.065	4.798	1.00	0.00	3A4
	MOTA	1137	С	ASP	193	49.942	0.941	3.982	1.00	0.00	3A4 3A4
	MOTA	1138	0	ASP	193	49.555 49.199	2.107 -0.025	4.042	1.00	0.00 0.00	3A4
	ATOM	1139 1140	N CA	SER SER	194 194	47.801	0.108	2.935	1.00	0.00	3A4
	ATOM ATOM	1141	CB	SER	194	47.674	0.859	1.564	1.00	0.00	3A4
	ATOM	1142	OG	SER	194	48.568	0.364	0.570	1.00	0.00	3A4
	MOTA	1143	С	SER	194	47.072	-1.263	2.877	1.00	0.00	3A4 3A4
	ATOM .	1144	0	SER	194	47.201	-1.949 -1.682	1.864 3.968	1.00	0.00	3A4
	ATOM	1145 1146	N CA	LEU	195 195	46.300 45.506	-2.928	4.205	1.00	0.00	3A4
	MOTA MOTA	1147	CB	LEU	195	44.616	-3.155	2.908	1.00	0.00	3A4
	ATOM	1148	CG	LEU	195	43.358	-4.046	2.893	1.00	0.00	3A4
•	ATOM	1149		LEU	195	42.566	-3.731	1.614	1.00	0.00	3A4 3A4
	ATOM	1150		LEU	195	43.591	-5.569 -4.231	2.963 4.384	1.00	0.00	3A4
	ATOM ATOM	1151 1152	С 0	LEU	195 195	46.313 46.823	-4.525	3.303	1.00	0.00	3A4
	ATOM	1152	N	ASN	196	46.462	-5.133	5.522	1.00	0.00	3A4
	ATOM	1154	CA	ASN	196	46.660	-6.447	5.007	1.00	0.00	3A4
	MOTA	1155	CB	ASN	196	48.141	-6.561	4.645	1.00	0.00	3A4 3A4
	MOTA	1156	CG.	ASN	196	48.532 49.287	-7.677 -8.581	3.641 3.992	1.00	0.00	3A4
	MOTA MOTA	1157 1158		ASN ASN	196 196	48.039	-7.601	2.374		0.00	3A4
	ATOM	1159	C	ASN	196	46.000	-7.578	5.603	1.00	0.00	3A4
	ATOM	1160	0	ASN	196	44.826	-7.879	5.338	1.00	0.00	3A4
	ATOM	1161	N	ASN	197	46.757	-8.297	6.407	1.00	0.00	3A4 3A4
	MOTA	1162	CA	ASN	197	46.317	-9.599 -10.511	6.859 7.443	1.00	0.00	3A4
	ATOM ATOM	1163 1164	CB CG	ASN ASN	197 197		-10.689	6.405	1.00	0.00	3A4
	ATOM	1165		ASN	197	48.334	-11.249	5.336	1.00	0.00	3A4
	MOTA	1166	ND2	ASN	197		-10.219	6.717	1.00	0.00	3A4 3A4
	ATOM	1167	C	ASN	197	45.160	-9.556	7.804 7.761	1.00	0.00	3A4
	ATOM	1168 1169	O N	ASN PRO	197 198	45.075	-10.439 -8.496	8.595	1.00	0.00	3A4
	MOTA MOTA	1170	CA	PRO	198	44.013	-8.420	9.555	1.00	0.00	3A4
	MOTA	1171	CD	PRO	198	46.277	-7.818	9.154	1.00		3A4
	MOTA	1172	СВ	PRO	198	44.652	-7.631	10.641	1.00		3A4 3A4
	ATOM	1173	CG	PRO	198	46.123 42.754	-7.908 -7.786	10.628 9.085			3A4
	MOTA MOTA	1174 1175	C O	PRO PRO	198 198	42.754		9.865			3A4
	MOTA	1176	N	GLN	199	42.701	-7.279	7.830	1.00	0.00	3A4
	ATOM	1177	CA	GLN	199	41.636		7.407			3A4
	ATOM	1178	СВ	GLN	199	41.900	-5.668	6.066			3A4 3A4
	MOTA	1179	CG	GLN	199	41.001 41.471	-4.419 -3.266				3A4
	ATOM ATOM	1180 1181	CD OE1	GLN GLN	199 199	42.353					3A4

ATOM	1182	NE2	GLN	199	40.885	-3.125	7.963	1.00	0.00	3A4
ATOM	1183	C	GLN	199	40.319	-7.071	7.338	1.00	0.00	3A4
MOTA	1184	0	GLN	199	39.374	-6.533	7.889	1.00	0.00	3A4 3A4
MOTA	1185	N	ASP	200	40.193 38.939	-8.262 -8.983	6.717 6.597	1.00	0.00	3A4
MOTA	1186 1187	CA CB	ASP ASP	200 200	39.049		5.538	1.00	0.00	3A4
ATOM ATOM	1188	CG	ASP	200	37.683 -		5.079	1.00	0.00	3A4
ATOM	1189	OD1		200	37.459 -		5.238	1.00	0.00	3A4
ATOM	1190	OD2	ASP	200	36.855	-9.893	4.566	1.00	0.00	3A4 3A4
MOTA	1191	C	ASP	200	38.347	-9.432	7.927 8.099	1.00	0.00	3A4
ATOM	1192	0	ASP	200 201	37.137 39.155	-9.315 -9.847	8.917	1.00	0.00	3A4
ATOM ATOM	1193 1194	N CA	PRO PRO	201	38.699		10.270	1.00	0.00	3A4
ATOM	1195	CD	PRO	201	40.343		8.654	1.00	0.00	3A4
ATOM	1196	СВ	PRO	201	39.936		11.012	1.00	0.00	3A4 3A4
MOTA	1197	CG	PRO	201	40.633		9.938 10.997	1.00	0.00	3A4
ATOM	1198	C	PRO	201 201	38.128 37.076	-8.916 -9.052	11.615	1.00	0.00	3A4
ATOM ATOM	1199 1200	O N	PRO PHE	202	38.762	-7.733	10.872	1.00	0.00	3A4
ATOM	1201	CA	PHE	202	38.319	-6.521	11.530	1.00	0.00	3A4
ATOM	1202	CB	PHE	202	39.462	-5.473	11.494	1.00	0.00	3A4 3A4
MOTA	1203	CG	PHE	202	40.009	-5.259	12.888	1.00	0.00 0.00	3A4
MOTA	1204		PHE	202	40.365 40.293	-6.366 -3.968	13.691 13.372	1.00	0.00	3A4
ATOM	1205 1206		PHE PHE	202 202	40.856	-6.184	14.987	1.00	0.00	3A4
ATOM ATOM	1207		PHE	202	40.855	-3.790	14.647	1.00	0.00	3A4
ATOM	1208	CZ	PHE	202	41.107	-4.894	15.465	1.00	0.00	. 3A4
ATOM	1209	С	PHE	202	37.080	-5.964	10.887	1.00	0.00 0.00	3A4 3A4
MOTA	1210	0	PHE	202	36.208 36.928	-5.444 -6.145	11.573 9.554	1.00	0.00	3A4
ATOM	1211 1212	N CA	VAL VAL	203 203	35.752	-5.762	8.799	1.00	0.00	3A4
ATOM ATOM	1212	CB	VAL	203	36.015	-5.808	7.287	1.00	0.00	3A4
ATOM	1214		VAL	203	34.738	-5.677	6.411	1.00	0.00	3A4
MOTA	1215		VAL	203	36.983	-4.648	6.954	1.00	0.00	3A4 3A4
ATOM	1216	C	VAL	203	34.545 33.451	-6.596 -6.068	9.199 9.364	1.00	0.00	3A4
ATOM	1217 1218	O N	VAL GLU	203 204	34.736	-7.908	9.475	1.00	0.00	3A4
ATOM ATOM	1219	CA	GLU	204	33.684	-8.782	9.967	1.00	0.00	3A4
ATOM	1220	СВ	GLU	204		-10.262	9.912	1.00	0.00	3A4 3A4
ATOM	1221	CG	GLU	204		-10.797	8.472	1.00	0.00	3A4
ATOM	1222	CD	GLU	204		-12.210 -12.394	8.489 7.934	1.00	0.00	3A4
ATOM ATOM	1223 1224		GLU	204 204		-13.123	9.059	1.00	0.00	3A4
MOTA	1225	C	GLU	204	33.230	-8.440	11.373	1.00	0.00	3A4
ATOM	1226	0	GLU	204	32.042		11.666	1.00	0.00	3A4 3A4
MOTA	1227	N	ASN	205	34.176	-8.057 -7.660	12.259 13.628	1.00	0.00	. 3A4
ATOM	1228	CA	ASN ASN	205 205	33.914 35.248	-7.438	14.383	1.00	0.00	3A4
MOTA MOTA	1229 1230	CB	ASN	205	36.015	-8.751	14.628	1.00	0.00	3A.4
ATOM	1231		ASN	205	37.233	-8.776	14.460	1.00	0.00	3A4
ATOM	1232	ND2	ASN	205	35.329	-9.842	15.069	1.00	0.00	3A4 3A4
MOTA	1233	c	ASN	205	33.087	-6.395 -6.344	13.736 14.487	1.00	0.00	3A4
MOTA MOTA	1234 1235	N O	ASN THR	205 206	32.115 33.414	-5.376	12.903	1.00		3A4
ATOM	1236	CA	THR	206	32.762	-4.077	12.899	1.00	0.00	3A4
ATOM	1237	СВ	THR	206	33.525	-3.007	12.102	1.00	0.00	3A4 3A4
MOTA	1238		THR	206	34.406	-3.549	11.139	1.00		3A4
MOTA	1239		THR	206 206	34.381 31.364	-2.246 -4.178	13.141	1.00		3A4
ATOM	1240 1241	C	THR THR	206	30.435	-3.581	12.843	1.00		3A4
MOTA MOTA	1241	N	LYS	207	31.178	-5.009	11.279	1.00		3A4
ATOM	1243	CA	LYS	207	29.905	-5.266	10.645	1.00		3A4 3A4
MOTA	1244	СВ	LYS	207	30.122	-6.061	9.349 8.393	1.00		3A4 3A4
ATOM	1245	CG	LYS	207 207	28.927 29.306	-6.211 -6.802	7.027			3A4
MOTA MOTA	1246 1247	CE	LYS LYS	207	29.832		7.088		0.00	3A4
ATOM	1248	NZ	LYS	207	30.150	-8.750	5.731			3A4
ATOM	1249	C	LYS	207	28.938					3A4 3A4
MOTA	1250		LYS	207	27.753					3A4 3A4
ATOM	1251	N	LYS	208	29.441 28.646			_		3A4
MOTA ATOM	1252 1253		LYS LYS	208 208	29.443					3A4
N I OM	1233	- 5	2,3							

ATOM	1254	CG	LYS	208	28.627	-9.993	14.610	1.00	0.00	3A4
ATOM	1255	CD	LYS	208	29.414	-11.248	15.031	1.00	0.00	3A4
ATOM	1256	CE	LYS	208	29.894		13.900	1.00	0.00	3A4 3A4
MOTA	1257	NZ	LYS	208	31.125 · 28.094	-6.905	13.236 14.430	1.00	0.00	3A4
MOTA	1258	С 0	LYS LYS	208 208	26.931	-7.047	14.780	1.00	0.00	3A4
ATOM ATOM	1259 1260	N	LEU	209	28.886	-5.983	15.022	1.00	0.00	3A4
ATOM	1261	CA	LEU	209	28.454	-5.149	16.133	1.00	0.00	3A4
ATOM	1262	CB	LEU	209	29.656	-4.415	16.784	1.00	0.00	3A4
MOTA	1263	CG	LEU	209	29.353	-3.397	17.945 19.146	1.00	0.00	3A4 3A4
ATOM	1264		LEU	209	28.592 30.596	-4.009 -2.606	18.399	1.00	0.00	3A4
ATOM	1265 1266	CD2	LEU	209 209	27.416	-4.112	15.737	1.00	0.00	3A4
ATOM ATOM	1267	0	LEU	209	26.515	-3.793	16.507	1.00	0.00	3A4
ATOM	1268	N	LEU	210	27.527	-3.561	14.510	1.00	0.00	3A4
ATOM	1269	CA	LEU	210	26.707	-2.449	14.080	1.00	0.00	3A4 3A4
ATOM	1270	СВ	LEU	210	27.559 28.684	-1.343 -0.850	13.418 14.384	1.00	0.00	3A4
ATOM	1271 1272	CG	LEU LEU	210 210	29.655	0.113	13.699	1.00	0.00	3A4
MOTA MOTA	1273		LEU	210	28.176	-0.257	15.717	1.00	0.00	3A4
ATOM	1274	c	LEU	210	25.611	-2.862	13.145	1.00	0.00	3A4
MOTA	1275	0	LEU	210	24.465	-2.454	13.335	1.00	0.00	3A4 3A4
ATOM	1276	N	ARG	211	25.948	-3.571 -3.650	12.035 10.816	1.00	0.00	3A4
ATOM	1277	CA	ARG ARG	211 211	25.146 26.033	-3.592	9.539	1.00	0.00	- 3A4
MOTA MOTA	1278 1279	CB CG	ARG	211	26.927	-2.337	9.503	1.00	0.00	3A4
ATOM	1280	CD	ARG	211	27.841	-2.220	8.274	1.00	0.00	3A4
ATOM	1281	NE	ARG	211	27.005	-2.107	7.024	1.00	0.00	3A4 3A4
MOTA	1282	CZ	ARG	211	26.814	-0.939	6.329 5.223	1.00	0.00	3A4
ATOM	1283		ARG	211 211	26.014 27.397	-0.951 0.236	6.711	1.00	0.00	3A4
ATOM ATOM	1284 1285	NH2 C	ARG ARG	211	24.236	-4.864	10.757	1.00	0.00	3A4
ATOM	1286	ō	ARG	211	23.275	-4.868	9.989	1.00	0.00	3A4
ATOM	1287	N	PHE	212	24.496	-5.910	11.589	1.00	0.00	3A4 3A4
ATOM	1288	CA	PHE	212	23.555	-6.992	11.826 10.930	1.00	0.00	3A4
ATOM	1289	CB	PHE PHE	212 212	23.730 25.061	-8.273 -8.998	10.938	1.00	0.00	3A4
ATOM ATOM	1290 1291	CG	PHE	212		-10.224	11.667	1.00	0.00	3A4
ATOM	1292		PHE	212	26.182	-8.527	10.268	1.00	0.00	3A4
ATOM	1293		PHE	212		-10.954	11.660	1.00	0.00	3A4 3A4
MOTA	1294		PHE	212	27.380	-9.259 -10.469	10.254	1.00	0.00	3A4
ATOM	1295	CZ C	PHE	212 212	23.608	-7.246	13.314	1.00	0.00	3A4
MOTA MOTA	1296 1297	Ö	PHE	212	24.292	-8.143		1.00	0.00	3A4
ATOM	1298	N	ASP	213		6.398	14.068		0.00	3A4
ATOM	1299	CA	ASP	213	22.843	-6.356	15.513	1.00	0.00	3A4 3A4
MOTA	1300	CB	ASP	213	23.642	-5.131 -5.215	16.046 17.558	1.00	0.00	3A4
MOTA MOTA	1301 1302	CG	ASP ASP	213 213	23.916 24.608	-6.179	17.982	1.00	0.00	3A4
ATOM	1302		ASP	213	23.444	-4.312	18.300	1.00	0.00	3A4
ATOM	1304	С	ASP	213	21.391	-6.281	15.902	1.00	0.00	3A4
ATOM	1305	0	ASP	213	20.714	-5.286	15.648	1.00	0.00	3A4 3A4
MOTA	1306	N	PHE	214	20.894 19.516	-7.371 -7.516	16.533 16.941	1.00	0.00	3A4
ATOM ATOM	1307 1308	CA CB	PHE	214 214	18.526	-7.900	15.776	1.00	0.00	3A4
ATOM	1309	CG	PHE	214	19.127		14.734	1.00	0.00	3A4
ATOM	1310	CD1	PHE	214	19.610	-8.306	13.515	1.00	0.00	3A4 3A4
ATOM	1311		PHE	214		-10.215 -9.143	14.950 12.550	1.00	0.00	3A4
ATOM	1312		PHE	214 214	20.186	-11.058	13.987	1.00	0.00	3A4
ATOM ATOM	1313 . 1314	CZ	PHE PHE	214		-10.520		1.00	0.00	3A4
ATOM	1315	Ċ	PHE	214	19.513	-8.554	18.034	1.00	0.00	3A4
ATOM	1316	0	PHE	214	20.344	-9.460	_	1.00		3A4 3A4
ATOM		N	LEU	215	18.527 18.216	-8.428 -9.384				3A4
ATOM		CA CB	LEU	215 215	18.216					3A4
MOTA MOTA			LEU	215		-10.089			0.00	3A4
ATOM			LEU	215	19.075	-11.533	22.128	1.00		3A4
MOTA	1322		LEU	215	19.419					3A4 3A4
MOTA			LEU	215	16.716 16.151					3A4
ATOM ATOM			LEU ASP	215 216	16.046					3A4
MULM	4-2-2	4.4		- - -						

ATOM	1326	CA	ASP	216	14.627	-9.830	18.781	1.00	0.00		3A4
ATOM	1327	СВ	ASP	216		-9.623	17.242	1.00	0.00		3A4
ATOM	1328	CG	ASP	216	14.915 -		16.328	1.00	0.00	•	3A4 3A4
ATOM	1329	ODI		216	16.161 -		16.241 15.700	1.00	0.00		3A4
MOTA	1330	OD2	ASP	216 216	14.075 - 13.914 -		19.316	1.00	0.00		3A4
ATOM ATOM	1331 1332	С 0	ASP	216	14.578 -		19.506	1.00	0.00		3A4
ATOM	1333	N	PRO	217	12.576 -		19.553	1.00	0.00		3A4
ATOM	1334	CA	PRO	217	11.794 -	12.227	19.974	1.00	0.00		3A4
MOTA	1335	CD	PRO	217		-9.819	19.695	1.00	0.00		3A4
MOTA	1336	СВ	PRO	217	10.525 ~		20.611 19.970	1.00	0.00		3A4 3A4
ATOM	1337	CG	PRO	217	10.367 - 11.504 -		18.786	1.00	0.00		3A4
ATOM ATOM	1338 1339	C	PRO PRO	217 217	12.309 -		18.527	1.00	0.00		3A4
ATOM	1340	N	PHE	218	10.374 -		18.064	1.00	0.00		3A4
ATOM	1341	CA	PHE	218	10.004 -		16.839	1.00	0.00		3A4
ATOM	1342	СВ	PHE	218	8.877 -		17.032	1.00	0.00		3A4 3A4
ATOM	1343	CG	PHE	218	9.294 -		18.036 19.273	1.00 1.00	0.00		3A4
MOTA	1344		PHE	218 218	8.630 - 10.354 -		17.766	1.00	0.00		3A4
ATOM ATOM	1345 1346		PHE	218	9.018 -		20.225	1.00	0.00		3A4
ATOM	1347		PHE	218	10.751 -		18.720	1.00	0.00		3A4
ATOM	1348	CZ	PHE	218	10.083 -		19.950	1.00	0.00		3A4
ATOM	1349	С	PHE	218	9.495 -		15.883	1.00	0.00		3A4 3A4
MOTA	1350	0	PHE	218	9.158 - 9.400 -		14.737 16.374	1.00	0.00		3A4
MOTA	1351 1352	N CA	PHE	219 219	8.762 -		15.736	1.00	0.00		3A4
ATOM ATOM	1352	CB	PHE	219	7.558	-9.630	16.572	1.00	0.00		3A4
ATOM	1354	CG	PHE	219	6.443 -	-10.646	16.570	1.00	0.00		3A4
ATOM	1355	CD1	PHE	219		-10.600	15.587	1.00	0.00		3A4
MOTA	1356		PHE	219		-11.664	17.542 15.576	1.00	0.00		3A4 3A4
ATOM	1357		PHE	219 219		-11.546 -12.611	17.536	1.00	0.00	•	3A4
ATOM ATOM	1358 1359	CZ CZ	PHE	. 219		-12.551	16.553	1.00	0.00		3A4
ATOM	1360	C	PHE	219	9.798	-9.078	15.602	1.00	0.00		3A4
ATOM	1361	0	PHE	219	10.805	-9.068	16.307	1.00	0.00		3A4
MOTA	1362	N	LEU	220	9.547	-8.131	14.664	1.00	0.00		3A4 3A4
MOTA	1363	CA	LEU	220	10.447 11.550	-7.050 -7.452	14.321 13.279	1.00	0.00		3A4
ATOM ATOM	1364 1365	CB CG	LEU	220 220	11.130	-7.889	11.840	1.00	0.00		· 3A4
ATOM	1366		LEU	220	12.368	-7.938		1.00	0.00		3A4
MOTA	1367		LEU	220	10.365	-9.229	11.764	1.00	0.00		3A4
MOTA	1368	С	LEU	220	9.590	-5.908	13.825	1.00	0.00		3A4 3A4
MOTA	1369	0	LEU	220	8.366	-5.964 -4.849	13.937 13.284	1.00	0.00		3A4
ATOM	1370 1371	N CA	SER	221 221	10.268 9.781	-3.584	12.735	1.00	0.00		3A4
ATOM ATOM	1372	CB	SER	221	8.270	-3.542	12.288	1.00	0.00		3A4
ATOM	1373	ŌĞ	SER	. 221	7,980	-2.485	11.376	1.00	0.00		3A4
MOTA	1374	С	SER	221	10.129	-2.514	13.764	1.00	0.00		3A4 3A4
MOTA	1375	0	SER	221	10.958	-2.740	14.646 13.661	1.00	0.00		3A4
ATOM	1376	N	ILE	222 222	9.495 9.692	-1.312 -0.155	14.524	1.00	0.00		3A4
ATOM ATOM	1377 1378	CA CB	ILE	222	9.886	1.145	13.735	1.00	0.00		3A4
ATOM	1379		ILE	222	11.258	1.038	13.025	1.00	0.00		3A4
MOTA	1380		ILE	222	8.727	1.449	12.741	1.00	0.00		3A4 3A4
ATOM	1381	CD	ILE	222	8.868	2.791	12.016 15.500	1.00	0.00		3A4
ATOM	1382	C	ILE	222	8.533 8.631	-0.038 0.670	16.501	1.00	0.00		3A4
MOTA MOTA	1383 1384	O N	ILE THR	222 223	7.406	-0.746	15.215	1.00	0.00		3A4
ATOM	1385	CA	THR	223	6.225	-0.787	16.050	1.00	0.00		3A4
ATOM	1386	СВ	THR	223	5.259	0.384	15.782	1.00	0.00		3A4
MOTA	1387		THR	223	4.159	0.414	16.691	1.00	0.00		3A4 3A4
ATOM	1388		THR	223	4.751 5.633	0.459 -2.165	14.318 15.811	1.00	0.00		3A4
ATOM	1389 1390	C O	THR THR		5.360	-2.558	14.678	1.00	0.00		3A4
MOTA MOTA	1391	N	VAL		5.435	-2.927	16.918	1.00	0.00		3A4
ATOM	1392	CA	VAL	224	4.832	-4.244	16.917		0.00		3A4
ATOM	1393	СВ	VAL		5.751	-5.354	16.379		0.00		3A4 3A4
MOTA	1394		VAL		7.065 4.973	-5.517 -6.679	17.186 16.198		0.00		3A4
ATOM ATOM	1395 1396	CG2	VAL VAL		4.397	-4.468	18.349		0.00		3A4
ATOM	1397	Ö	VAL		5.085	-4.071	19.290		0.00		3A4

ATOM	1398	N	PHE	225	3.212 -5.11	18.534	1.00	0.00	3A4
ATOM	1399	CA	PHE	225	2.568 -5.39	8 19.809	1.00	0.00	3A4
ATOM	1400	СВ	PHE	225	1.025 -5.11		1.00	0.00	3A4
ATOM	1401	CG .	PHE	225	0.345 -5.08		1.00	0.00	3A4
MOTA	1402	CD1		225	0.584 -4.03		1.00	0.00	3A4 3A4
MOTA	1403	CD2		225	-0.533 -6.12		1.00	0.00	3A4
MOTA	1404	CE1		225	-0.038 -4.01		1.00	0.00	3A4
ATOM	1405	CE2		225	-1.156 -6.10 -0.908 -5.0		1.00	0.00	3A4
ATOM	1406	CZ	PHE	225 225	2.898 -6.81		1.00	0.00	3A4
ATOM	1407 1408	С 0	PHE	225	3.306 -6.88		1.00	0.00	3A4
MOTA MOTA	1409	N	PRO	226	2.776 -7.9		1.00	0.00	3A4
ATOM	1410	CA	PRO	226	3.087 -9.29		1.00	0.00	3A4
ATOM	1411	CD	PRO	226	2.027 -8.0	62 18.335	1.00	0.00	3A4
ATOM	1412	СВ	PRO	226	2.324 -10.2	68 19.186	1.00	0.00	3A4
ATOM	1413	CG	PRO	226	2.191 -9.50		1.00	0.00	3A4
ATOM	1414	С	PRO	226	4.587 -9.5		1.00	0.00	3A4
ATOM	1415	0	PRO	226	5.346 -9.0		1.00	0.00	3A4 3A4
MOTA	1416	N	PHE	227	4.993 -10.5		1.00	0.00	3A4
ATOM	1417	CA	PHE	227	6.356 -10.9		1.00	0.00	3A4
MOTA	1418	CB	PHE	227	7.106 -10.25 6.298 -10.15		1.00	0.00	3A4
MOTA		CG	PHE	227 227	5.437 -9.0		1.00	0.00	3A4
ATOM	1420 1421	CD1	PHE	227	6.393 -11.1		1.00	0.00	3A4
ATOM ATOM	1422		PHE	227	4.677 -8.9		1.00	0.00	3A4
ATOM	1423		PHE	227	5.634 -10.9		1.00	0.00	3A4
ATOM	1424	cz	PHE	227	4.775 -9.9		1.00	0.00	3A4
ATOM	1425	C	PHE	227	6.307 -12.4		1.00	0.00	3A4
ATOM	1426	0	PHE	227	7.291 -13.1		1.00	0.00	3A4
MOTA	1427	N	LEU	228	5.134 -13.0		1.00	0.00	3A4
ATOM	1428	CA	LEU	228	4.753 -14.3		1.00	0.00	3A4 3A4
ATOM.	1429	СВ	LEU	228	5.137 -15.3		1.00	0.00	3A4
ATOM	1430	CG	LEU	228	4.217 -16.6		1.00	0.00	3A4
ATOM	1431		LEU	228	4.267 -17.7 2.767 -16.2		1.00	0.00	3A4
MOTA	1432		LEU	228 228	5.274 -14.7		1.00	0.00	3A4
MOTA	1433 1434	С 0	LEU	228	4.778 -14.2		1.00	0.00	3A4
ATOM ATOM	1435	N	ILE	229	6.316 -15.6		1.00	0.00	3A4
ATOM	1436	CA	ILE	229	7.097 -15.9		1.00	0.00	3A4
ATOM	1437	СВ	ILE	229	6.457 -16.9	44 25.799	1.00	0.00	3A4
ATOM	1438		ILE	229	6.056 -18.3		1.00	0.00	3A4
MOTA	1439	CG1	ILE	229	7.185 -17.0		1.00	0.00	3A4
ATOM	1440	CD	ILE	229	8.372 -18.0		1.00	0.00	3A4 3A4
MOTA	1441	С	ILE	229	8.458 -16.3		1.00	0.00	3A4
MOTA	1442	0	ILE	229	8.631 -17.5		1.00	0.00	3A4
ATOM	1443	N	PRO	230	9.474 -15.4 10.759 -15.7		1.00	0.00	 3A4
ATOM	1444	CA	PRO	230 230	9.306 -14.0		1.00	0.00	3A4
MOTA MOTA	1445 1446	CD CB	PRO PRO	230	11.244 -14.3			0.00	3A'4
MOTA	1447	CG	PRO	230	10.655 -13.3		1.00	0.00	3A4
ATOM	1448	ç	PRO	230	11.749 -16.3	80 24.483	1.00	0.00	3A4
ATOM	1449	ō	PRO	230	11.509 -16.4		1.00	0.00	3A4
ATOM	1450	N	ILE	231	12.894 -16.8	70 23.931	1.00	0.00	3A4
ATOM	1451	CA	ILE	231	13.997 -17.4	95 24.644		0.00	3A4
MOTA	1452	CB	ILE	231	14.463 -18.8			0.00	3A4 3A4
MOTA	1453		ILE	231	15.554 -19.4			0.00	3A4
ATOM	1454		ILE	231	13.275 -19.7			0.00	3A4
MOTA	1455	CD	ILE	231	12.502 -20.2 15.116 -16.4			0.00	3A4
ATOM	1456	C	ILE	231 231	15.691 -16.2			0.00	3A4
ATOM	1457	N O	ILE LEU	232	15.428 -15.8			0.00	3A4
ATOM ATOM	1458 1459	CA	LEU	232	16.397 -14.7			0.00	3A4
MOTA	1460	CB	LEU	232	16.312 -13.5			0.00	3A4
ATOM	1461	CG	LEU		14.944 -12.8	324 24.269		0.00	3A4
ATOM	1462		LEU	232	14.900 -11.	763 25.383		0.00	3A4
ATOM	1463		LEU	232	14.567 -12.2			0.00	3A4
MOTA	1464	С	LEU	232	17.814 -15.			0.00	3A4
ATOM	1465	0	LEU	232	18.606 -15.			0.00	3A4 3A4
MOTA	1466	N	GLU	233	18.131 -16.0			0.00	3A4
MOTA	1467	CA	GLU	233	19.390 -16.				3A4
ATOM	1468	CB	GLU	233	19.269 -18.3 18.095 -18.				3A4
MOTA	1469	CG	GLU	233	10.033 -10.	,,, ex.,,,		5.00	

ATOM	1470	CD	GLU	233	18.120 -20.462 21.648 1.00 0.00	3A4
MOTA	1471	OE1		233	19.140 -21.114 21.295 1.00 0.00 17.118 -20.985 22.205 1.00 0.00	3A4 3A4
ATOM	1472	OE2	GLU GLU	233 233	17.118 -20.985 22.205 1.00 0.00 19.828 -16.395 20.489 1.00 0.00	3A4
ATOM ATOM	1473 1474	С О	GLU	233	20.256 -17.261 19.726 1.00 0.00	3A4
ATOM	1475	N	VAL	234	19.734 -15.088 20.125 1.00 0.00	3A4
MOTA	1476	CA	VAL	234	20.053 -14.558	3A4 3A4
ATOM	1477	CB	VAL	234 234	18.792 -14.275 17.987 1.00 0.00 17.739 -13.402 18.723 1.00 0.00	3A4
ATOM ATOM	1478 1479	CG1		234	19.142 -13.768 16.568 1.00 0.00	3A4
ATOM	1480	c	VAL	234	20.960 -13.370 19.064 1.00 0.00	3A4
ATOM	1481	0	VAL	234	20.563 -12.209 18.984 1.00 0.00 22.242 -13.673 19.393 1.00 0.00	3A4 3A4
ATOM	1482	N	LEU	235 235	22.242 -13.673	3A4
MOTA MOTA	1483 1484	CA CB	LEU	235	23.137 -11.954 21.056 1.00 0.00	3A4
ATOM	1485	CG	LEU	235	23.294 -12.749 22.393 1.00 0.00	3A4
MOTA	1486		LEU	235	23.236 -11.785 23.594 1.00 0.00 22.289 -13.903 22.600 1.00 0.00	3A4 3A4
ATOM	1487		LEU	235 235	22.289 -13.903 22.600 1.00 0.00 24.592 -13.413 19.593 1.00 0.00	3A4
ATOM ATOM	1488 1489	С 0	LEU	235	24.703 -14.586 19.948 1.00 0.00	3A4
ATOM	1490	N	ASN	236	25.638 -12.684 19.128 1.00 0.00	3A4
ATOM	1491	CA	ASN	236	27.013 -13.135	3A4 3A4
MOTA	1492	CB	ASN	236	27.351 -13.966 17.803 1.00 0.00 28.697 -14.706 17.931 1.00 0.00	3A4
ATOM ATOM	1493 1494	CG OD1	ASN ASN	236 236	28.818 -15.613 18.753 1.00 0.00	3A4
ATOM	1495		ASN	236	29.719 -14.326 17.115 1.00 0.00	3A4
ATOM	1496	C	ASN	236	27.795 -11.845 19.165 1.00 0.00 28.546 -11.489 18.259 1.00 0.00	3A4 3A4
ATOM	1497	0	ASN	236	28.546 -11.489 18.259 1.00 0.00 27.590 -11.096 20.283 1.00 0.00	3A4
ATOM ATOM	1498 1499	N CA	ILE ILE	237 237	28.074 -9.747 20.504 1.00 0.00	3A4
ATOM	1500	СВ	ILE	237	26.980 -8.800 20.998 1.00 0.00	3A4
MOTA	1501		ILE	237	26.039 -8.584 19.789 1.00 0.00 26.203 -9.271 22.262 1.00 0.00	3A4 3A4
ATOM	1502		ILE	237	26.203 -9.271 22.262 1.00 0.00 25.059 -8.341 22.671 1.00 0.00	3A4
ATOM ATOM	1503 1504	CD	ILE ILE	237 237	29.228 -9.798 21.461 1.00 0.00	3A4
ATOM	1505	ŏ	ILE	237	30.202 -9.126 21.226 1.00 0.00	3A4
MOTA	1506	N	CYS	238	29.124 -10.614 22.532 1.00 0.00 30.099 -10.834 23.576 1.00 0.00	3A4 3A4
ATOM	1507	CA	CYS	238	30.099 -10.834 23.576 1.00 0.00 29.513 -11.689 24.739 1.00 0.00	3A4
MOTA MOTA	1508 1509	CB SG	CYS	238 238	28.106 -10.870 25.526 1.00 0.00	3A4
ATOM	1510	c	CYS	238	31.307 -11.563 23.083 1.00 0.00	3A4
ATOM	1511	0	CYS	238	32.424 -11.278 23.493 1.00 0.00 31.138 -12.446 22.082 1.00 0.00	3A4 3A4
ATOM	1512	N	VAL	239 239	31.138 -12.446 22.082 1.00 0.00 32.219 -13.161 21.438 1.00 0.00	3A4
ATOM ATOM	1513 1514	CA CB.	VAL VAL	239	31.700 -14.367 20.675 1.00 0.00	3A4
ATOM	1515		VAL	239	32.858 -15.308 20.247 1.00 0.00	3A4
ATOM,	1516		VAL	239	30.715 -15.139 21.586 1.00 0.00 33.006 -12.283 20.505 1.00 0.00	3A4 3A4
ATOM	1517	C	VAL VAL	239 239	33.006 -12.283	3A4
ATOM ATOM	1518 1519	N O	PHE	240	32.315 -11.420 19.731 1.00 0.00	3A4
ATOM	1520	CA	PHE	240	32.913 -10.422 18.870 1.00 0.00	3A4 3A4
ATOM	1521	СВ	PHE	240	31.825 -9.669 18.040 1.00 0.00 31.881 -8.134 17.899 1.00 0.00	3A4
ATOM	1522 1523	CG	PHE	240 240	31.881 -8.134 17.899 1.00 0.00 32.913 -7.550 17.149 1.00 0.00	3A4
MOTA MOTA	1524		PHE	240	31.185 -7.320 18.812 1.00 0.00	3A4
ATOM	1525		PHE	240	33.312 -6.223 17.382 1.00 0.00	3A4 3A4
MOTA	1526		PHE	240	31.646 -6.034 19.117 1.00 0.00 32.709 -5.481 18.396 1.00 0.00	3A4
ATOM ATOM	1527 1528	CZ C	PHE	240 240	33.789 -9.440 19.608 1.00 0.00	3A4
ATOM	1529	ŏ	PHE	240	34.906 -9.202 19.168 1.00 0.00	3A4
ATOM	1530	N	PRO	241	33.347 -8.835 20.727 1.00 0.00 34.111 -7.940 21.493 1.00 0.00	3A4 3A4
MOTA	1531	CA	PRO	241	34.111 -7.940 21.493 1.00 0.00 32.648 -9.345 21.724 1.00 0.00	3A4
ATOM ATOM	1532 1533	CD CB	PRO PRO	241 241	33.196 -7.358 22.578 1.00 0.00	3A4
MOTA	1534	CG	PRO	241	32.348 -8.435 22.936 1.00 0.00	3A4
ATOM	1535	С	PRO		35.347 -8.605 22.103 1.00 0.00 36.396 -7.992 22.029 1.00 0.00	3A4 3A4
ATOM	1536		PRO		36.396 -7.992 22.029 1.00 0.00 35.316 -9.867 22.592 1.00 0.00	3A4
MOTA MOTA	1537 1538	N CA	ARG ARG		36.450 -10.583 23.101 1.00 0.00	3A4
ATOM	1539		ARG		35.986 -11.889 23.750 1.00 0.00	3A4
MOTA	1540	CG	ARG	242	35.213 -11.657 25.054 1.00 0.00 34 515 -12.928 25.556 1.00 0.00	3A4 3A4
MOTA	1541	CD	ARG	242	34.515 -12.928 25.556 1.00 0.00	7117

ATOM	1542	NE	ARG	242	33.717 -	12.581	26.784	1.00	0.00	3A4
ATOM	1543	CZ	ARG	242	32.762 -		27.314		0.00	3A4
MOTA	1544	NH1.	ARG	242	32.114 -		28.455		0.00	3A4 3A4
MOTA	1545	NH2		242	32.444 -		26.725		0.00	3A4
MOTA	1546	С	ARG	242	37.483 -		22.037 22.298		0.00	3A4
MOTA	1547	0	ARG	242 243	38.677 - 37.044 -		20.784	1.00	0.00	3A4
MOTA	1548 1549	N CA	GLU	243	37.911 -		19.638	1.00	0.00	3A4
ATOM ATOM	1550	CB	GLU	243	37.126 -		18.383	1.00	0.00	3A4
ATOM	1551	CG	GLU	243	36.626 -	13.298	18.452	1.00	0.00	3A4
ATOM	1552	CD	GLU	243	35.759 -		17.219	1.00	0.00	3A4
ATOM	1553	OEl		243	34.528 -		17.385	1.00	0.00	3A4 3A4
ATOM	1554	OE2		243	36.319 - 38.703 -		16.089 19.275	1.00	0.00	3A4
MOTA	1555	C	GLU	243 243	39.908 -		19.057	1.00	0.00	3A4
ATOM ATOM	1556 1557	O N	GLU VAL	244		-8.981	19.287	1.00	0.00	3A4
ATOM	1558	CA	VAL	244		-7.714	18.990	1.00	0.00	3A4
ATOM	1559	СB	VAL	244		-6.607	18.731	1.00	0.00	3A4
ATOM	1560		VAL	244		-5.314	18.259	1.00	0.00	· 3A4 3A4
MOTA	1561		VAL	244	36.813	-7.052	17.545 20.084	1.00	0.00	3A4
MOTA	1562	C	VAL	244	39.649 40.771	-7.327 -6.912	19.811	1.00	0.00	3A4
ATOM	1563 1564	O N	VAL THR	244 245	39.257	-7.535	21.357	1.00	0.00	3A4
MOTA MOTA	1565	CA	THR	245	40.070	-7.264	22.527	1.00	0.00	3A4
ATOM	1566	СВ	THR	245	39.245	-7.434	23.795	1.00	0.00	3A4
ATOM	1567		THR	245	38.211	-6.455	23.817	1.00	0.00	3A4
MOTA	1568	CG2	THR	245	40.041	-7.330	25.127	1.00	0.00	3A4 3A4
MOTA	1569	С	THR	245	41.317	-8.113	22.572 22.842	1.00	0.00	3A4
ATOM	1570	0	THR	245	42.397 41.225	-7.605 -9.408	22.207	1.00	0.00	3A4
MOTA	1571 1572	N CA	ASN ASN	246 246	42.344 -		22.152	1.00	0.00	3A4
ATOM ATOM	1573	CB	ASN	246	41.877 -		21.874	1.00	0.00	3A4
ATOM	1574	CG	ASN	246	41.116 -		23.082	1.00	0.00	3A4
MOTA	1575	OD1	ASN	246	41.128 -		24.187	1.00	0.00	3A4 3A4
MOTA	1576		ASN.	246	40.427 -		22.862	1.00	0.00	3A4
MOTA	1577	C	ASN	246	43.340. 44.544 -		21.088	1.00	0.00	3A4
MOTA	1578	N 0	ASN PHE	246 247	42.846	-9.491	19.921	1.00	0.00	3A4
MOTA MOTA	1579 1580	CA	PHE	247	43.640	-9.006	18.820	1.00	0.00	3A4
ATOM	1581	СВ	PHE	247	42.712	-8.691	17.625	1.00	0.00	3A4
ATOM	1582	CG	PHE	247	43.520	-8.335	16.378	1.00	0.00	3A4 3A4
MOTA	1583		PHE	247	44.084	-9.348		1.00	0.00	3A4
MOTA	1584		PHE		43.817 44.943	-6.990 -9.028	16.065	1.00	0.00	3A4
ATOM	1585		PHE	247 247	44.673	-6.665	15.008	1.00	0.00	3A4
ATOM ATOM	1586 1587	CZ	PHE	247	45.245	-7.686	14.243	1.00	0.00	3A4
MOTA	1588	c	PHE	247	44.438	-7.768	19.171	1.00	0.00	3A4
ATOM	1589	0	PHE	247	45.631	-7.693	18.897	1.00	0.00	3A4 3A4
MOTA	1590	N	LEU	248	43.781	-6.766	19.795	1.00	0.00	. 3A4
MOTA	1591	CA	LEU	248 248	44.374 43.291	-5.480 -4.473	20.131 20.599	1.00	0.00	3A4
ATOM	1592 1593	CB CG	LEU	248	42.423	-3.985	19.422	1.00	0.00	3A4
MOTA MOTA	1594		LEU	248	41.143	-3.318	19.920	1.00	0.00	3A4
ATOM	1595		LEU	248	43.179	-3.055	18.448	1.00	0.00	3A4
ATOM	1596	С	LEU	248	45.407	-5.587	21.219	1.00	0.00	3A4 3A4
MOTA	1597	0	LEU	248	46.458	-4.959	21.175	1.00	0.00	3A4
ATOM	1598	N	ARG	249	45.152	-6.483 -6.805	22.189 23.263	1.00	0.00	3A4
ATOM	1599	CA	ARG ARG	249 249	46.055 45.402	-7.886	24.160	1.00	0.00	3A4
MOTA MOTA	1600 1601	CB	ARG	249	44.526	-7.297	25.274	1.00	0.00	3A4
MOTA	1602	CD	ARG	249	45.372	-6.731	26.426		0.00	3A4
ATOM	1603	NE	ARG	249	44.462	-6.210	27.502		0.00	3A4 3A4
ATOM	1604	CZ	ARG		44.932	-5.795	28.722		0.00	3A4 3A4
ATOM	1605		ARG		44.068	-5.248 -5.917	29.621 29.056		0.00	3A4
ATOM	1606		ARG		46.251 47.418	-7.301	22.846		0.00	3A4
ATOM ATOM	1607 1608	C	ARG ARG		48.444	-6.897	23.385		0.00	3A4
ATOM	1609	N	LYS		47.456	-8.139	21.790	1.00		3A4
ATOM	1610	CA	LYS		48.664	-8.643				3A4
ATOM	1611	CB	LYS		48.353	-9.760				. 3A4 3A4
ATOM	1612	CG	LYS			-11.007				3A4
ATOM	1613	CD	LYS	250	4/.184	-11.995	17.13			

АТОН	1614	CE	LYS	250	46.472	-13.190	20.404	1.00	0.00	3A4
ATOM	1615	NZ	LYS	250		-14.102	19.372	1.00	0.00	3A4
ATOM	1616	С	LYS	250	49.481	-7.572	20.506	1.00	0.00	3A4 3A4
MOTA	1617	Õ	LYS	250	50.699 48.809	-7.572 -6.584	20.583	1.00	0.00	3A4
ATOM	1618	N	SER	251 251	49.413	-5.423	19.268	1.00	0.00	3A4
ATOM ATOM	1619 1620	CA CB	SER SER	251	48.350	-4.598	18.498	1.00	0.00	3A4
ATOM	1621	OG	SER	251	47.705	-5.410	17.524	1.00	0.00	3A4
ATOM	1622	C	SER	251	50.056	-4.492	20.271	1.00	0.00	3A4
MOTA	1623	0	SER	251	51.163	-4.000	20.091	1.00	0.00	3A4
ATOM	1624	N	VAL	252	49.376	-4.275	21.416 22.495	1.00	0.00	3A4 3A4
ATOM	1625	CA	VAL	252 252	49.809 48.673	-3.398 -3.198	23.486	1.00	0.00	3A4
ATOM ATOM	1626 1627	CB CG1	VAL VAL	252	49.132	-2.497	24.775	1.00	0.00	3A4
ATOM	1628		VAL	252	47.610	-2.462	22.625	1.00	0.00	3A4
ATOM	1629	С	VAL	252	51.052	-3.938	23.163	1.00	0.00	3A4
MOTA	1630	0	VAL	252	51.998	-3.206	23.419	1.00	0.00	3A4 3A4
ATOM	1631	N	LYS	253	51.108		23.380 23.944	1.00	0.00	3A4
ATOM	1632	CA	LYS	253 253	52.243 51.887	-5.976 -7.462	24.155	1.00	0.00	3A4
ATOM ATOM	1633 1634	CB CG	LYS LYS	253	52.903	-8.297	24.953	1.00	0.00	3A4
ATOM	1635	CD	LYS	253	52.410	-9.721	25.224	1.00	0.00	3A4
ATOM	1636	CE	LYS	253		-10.563	26.018	1.00	0.00	3A4
ATOM	1637	NZ	LYS	253		-11.929	26.256	1.00	0.00	3A4 3A4
ATOM	1638	С	LYS	253	53.481	-5.877 -5.578	23.082 23.557	1.00	0.00 0.00	3A4
ATOM	1639	0	LYS ARG	253 254	54.570 53.316	-6.057	21.752	1.00	0.00	3A4
ATOM ATOM	1640 1641	N CA	ARG	254	54.372	-5.928	20.768	1.00	0.00	3A4
ATOM	1642	СВ	ARG	254	53.887	-6.368	19.369	1.00	0.00	3A4
ATOM	1643	CG	ARG	254	53.631	-7.877	19.278	1.00	0.00	3A4
MOTA	1644	CD	ARG	254	52.822	-8.252	18.031	1.00	0.00	3A4 3A4
ATOM	1645	NE	ARG	254	52.473	-9.714 -10.256	18.098 17.466	1.00	0.00	3A4
ATOM ATOM	1646 1647	CZ NH1	ARG ARG	254 254		-11.591	17.596	1.00	0.00	3A4
ATOM	1648		ARG	254	50.529	-9.490	16.721	1.00	0,.00	3A4
ATOM	1649		ARG	254	54.899	-4.517	20.676	1.00	0.00	3A4
ATOM	1650	0	ARG	254	56.093	-4.310	20.498	1.00	0.00	3A4
MOTA	1651	N	MET		54.021	-3.508	20.844	1.00	0.00	3A4 3A4
ATOM	1652	CA	MET	255	54.372 53.141	-2.106 -1.258	20.777	1.00	0.00	3A4
ATOM ATOM	1653 1654	CB CG	MET MET	255 255	52.816	-1.403	18.917	1.00	0.00	3A4
ATOM	1655	SD	MET	255	51.250	-0.639	18.447	1.00	0.00	3A4
ATOM	1656	CE	MET	255	51.470	-0.681	16.649	1.00	0.00	3A4
ATOM	1657	C	MET	255	55.008	-1.583	22.041	1.00	0.00	3A4
MOTA	1658	0	MET	255	55.687	-0.563 -2.296	22.027 23.174	1.00	0.00	3A4 3A4
ATOM	1659 1660	N CA	LYS LYS	256 256	54.853 55.524	-1.998	24.424	1.00	0.00	3A4
ATOM ATOM	1661	CB	LYS	256	54.809	-2.661	25.623	1.00	0.00	3A4
ATOM	1662	CG	LYS	256	53.537	-1.942	26.076	1.00	0.00	3A4
MOTA	1663	CD	LYS	256	52.726	-2.649	27.168	1.00	0.00	3A4
ATOM	1664	CE	LYS	256	53.383	-2.616 -3.206	28.556	1.00	0.00	3A4 3A4
ATOM	1665 1666	NZ C	LYS LYS	256 256	52.487 56.960	-2.488	29.579 24.397	1.00	0.00	3A4
ATOM ATOM	1667	Ö	LYS	256	57.837		25.029		0.00	3A4
ATOM	1668	N	GLU	257	57.220	-3.565	23.619	1.00	0.00	3A4
MOTA	1669	CA	GLU	257	58.527		23.444	1.00	0.00	3A4
MOTA	1670	СB	GLU	257	58.421		23.058	1.00	0.00	3A4 3A4
ATOM	1671	CG	GLU	257 257	57.813 57.607		24.182 23.679	1.00	0.00	3A4
ATOM ATOM	1672 1673	CD OF1	GLU GLU	257	56.428		23.604	1.00	0.00	3A4
ATOM	1674		GLU	257	58.625		23.363	1.00	0.00	3A4
ATOM	1675	C	GLU	257	59.381	-3.451	22.410	1.00	0.00	3A4
ATOM	1676	0	GLU	257	60.407		22.760	1.00	0.00	3A4
ATOM	1677	N	SER	258	59.003		21.108 20.026	1.00	0.00	3A4 3A4
ATOM	1678	CA CB	SER SER	258 258	59.766 61.186		19.807	1.00	0.00	3A4
MOTA MOTA	1679 1680	OG	SER	258	62.002		18.899	1.00	0.00	3A4
ATOM	1681	c	SER	258	58.938		18.776	1.00	0.00	3A4
ATOM	1682	o	SER	258	58.503	-4.225	18.459	1.00	0.00	3A4
ATOM	1683	N	ARG	259	58.779		18.007	1.00	0.00	3A4 3A4
MOTA	1684	CA	ARG	259	58.391		16.612 16.329	1.00	0.00	3A4
ATOM	1685	CB	ARG	259	56.880	-1.136	10.363	1.00		

ATOM	1686	CG	ARG	259	55.968	-2.939	16.688	1.00	0.00	3A4
ATOM	1687	CD	ARG	259	54.607	-2.858	15.987	1.00	0.00	3A4
ATOM	1688	NE	ARG	259	53.744	-4.000	16.458	1.00	0.00	3A4
ATOM	1689	CZ	ARG	259	52.617	-4.411	15.791	1.00	0.00	3A4
ATOM	1690	NH1	ARG	259	51.837	-5.390	16.332	1.00	0.00	3A4
ATOM	1691	NH2	ARG	259	52.247	-3.859	14.598	1.00	0.00	3A4
ATOM	1692	С	ARG	259	59.262	-0.943	16.000	1.00	0.00	3A4
ATOM	1693	0	ARG	259	60.401	-1.220	15.626	1.00	0.00	3A4
MOTA	1694	N	LEU	260	58.752	0.314	15.898	1.00	0.00	3A4
ATOM	1695	CA	LEU	260	59.502	1.436	15.373	1.00	0.00	3A4
MOTA	1696	CB	LEU	260	59.602	1.425	13.811	1.00	0.00	3A4 3A4
ATOM	1697	CG	LEU	260	60.595	2.428	13.175	1.00	0.00	3A4
MOTA	1698	CD1		260	62.054	2.163	13.599	1.00	0.00	3A4
ATOM	1699		LEU	260	60.467	2.427	11.640	1.00	0.00	3A4
MOTA	1700	C	LEU	260	58.790	2.670	15.874	1.00	0.00	3A4
MOTA	1701	0	LEU	260	58.005	3.291	15.159 17.155	1.00	0.00	3A4
MOTA	1702	N	GLU	261	59.062	3.038	17.133	1.00	0.00	3A4
MOTA	1703	CA	GLU	261	58.441	4.130 3.683	19.213	1.00	0.00	3A4
MOTA	1704	CB	GLU	261	57.742 58.554	2.841	20.229	1.00	0.00	3A4
MOTA	1705	CG	GLU	261	58.717	1.386	19.761	1.00	0.00	3A4
MOTA	1706	CD	GLU	261 261		0.942	19.589	1.00	0.00	3A4
MOTA	1707		GLU	261	57.675	0.701	19.572	1.00	0.00	3A4
ATOM	1708		GLU	261	59.482	5.186	18.166	1.00	0.00	3A4
ATOM	1709 1710	С О	GLU	261	60.619	4.877	18.523	1.00	0.00	3A4
ATOM ATOM	1711	N	ASP	262	59.067	6.478	17.991	1.00	0.00	3A4
ATOM	1712	CA	ASP	262	59.771	7.738	18.239	1.00	0.00	3A4
ATOM	1713	СВ	ASP	262	60.392	7.859	19.674	1.00	0.00	3A4
ATOM	1714	CG	ASP	262	59.293	7.671	20.735	1.00	0.00	3A4
ATOM	1715	OD1		262	59.392	6.700	21.533	1.00	0.00	3A4
ATOM	1716		ASP	262	58.341	8.497	20.759	1.00	0.00	3A4
ATOM	1717	С	ASP	262	60.828	8.011	17.175	1.00	0.00	3A4
ATOM	1718	0	ASP	262	62.015	8.125	17.477	1.00	0.00	3A4
ATOM	1719	Ν.	THR	263	60.385	8.087	15.889	1.00	0.00	3A4
ATOM	1720	CA	THR	263 ·	61.231	8.151	14.709	1.00	0.00	3A4 3A4
ATOM	1721	CB	THR	263	61.257	6.828	13.922	1.00	0.00	3A4
MOTA	1722		THR	263	59.962	6.247	13.768	1.00	0.00	3A4
ATOM	1723	CG2		263	62.163	5.831	14.677	1.00	0.00	3A4
MOTA	1724	С	THR	263	60.819	9.346	13.857 14.127	1.00	0.00	3A4
ATOM	1725	0	THR	263	61.248	10.466 9.120	12.773	1.00	0.00	3A4
MOTA	1726	N	GLN	264	60.017 - 59.831	10.032	11.649	1.00	0.00	3A4
MOTA	1727	CA	GLN	264 264	59.812	9.263	10.288	1.00	0.00	3A4
ATOM	1728	CB	GLN	264	61.018	8.324	10.094	1.00	0.00	3A4
MOTA	1729 1730	CD	GLN	264	60.951	7.671	8.710	1.00	0.00	3A4
ATOM ATOM	1731	OE1		264	61.775	7.968	7.846	1.00	0.00	3A4
ATOM	1732		GLN	264	59.961	6.763	8.489	1.00	0.00	3A4
ATOM	1733	C	GLN	264	58.564	10.861	11.768	1.00	0.00	3A4
ATOM	1734	ŏ	GLN	264	57.907	10.891	12.808	.1.00	0.00	3A4
ATOM	1735	N	LYS	265	58.214	11.556	10.645	1.00	0.00	3A4
MOTA	1736	CA	LYS	265	57.091	12.459	10.453	1.00	0.00	3A4
MOTA	1737	CB	LYS	265	57.471	13.608	9.470	1.00	0.00	3A4
MOTA	1738	CG	LYS	265	56.414	14.703	9.209	1.00	0.00	3A4 3A4
ATOM	1739	CD	LYS	265	55.986	15.485	10.458	1.00	0.00	3A4
MOTA	1740	CE	LYS	265	55.004	16.618	10.140	1.00		3A4
ATOM	1741	ΝZ	LYS	265	54.585	17.323	11.374	1.00	0.00	3A4
MOTA	1742	С	LYS	265	55.895	11.698	9.920	1.00	0.00	3A4
MOTA	1743	0	LYS	265	54.757	11.957 10.712	10.308 9.017	1.00	0.00	3A4
MOTA	1744	N	HIS	266	56.161 55.192	9.789	8.453	1.00	0.00	3A4
ATOM	1745	CA	HIS	266	53.192	11.484	6.555	1.00	0.00	3A4
ATOM	1746		HIS	266 266	54.551	11.168	6.457	1.00	0.00	3A4
ATOM	1747	CG	HIS HIS	266	55.138	9.857	6.906		0.00	3A4
ATOM	1748 1749	CB NE2	HIS	266	54.234	13.294	5.769	1.00	0.00	3A4
MOTA MOTA	1750		HIS	266	55.161	12.287	5.977		0.00	3A4
ATOM	1751		HIS	266	53.080	12.764	6.128		0.00	3A4
MOTA	1752	C	HIS	266	55.520	8.402	8.961		0.00	3A4
ATOM	1753	ŏ	HIS		55.595	7.432	8.208	1.00	0.00	3A4
ATOM	1754	N	ARG		55.681	8.319	10.306			3A4
ATOM	1755	CA	ARG		55.78 7	7.112				3A4
ATOM	1756	СВ	ARG		57.206	6.450				3A4
MOTA	1757	CG	ARG	267	57.342	5.024	11.602	1.00	0.00	3A4

ATOM	1758	CD	ARG	267	56.433	3.983	10.915	1.00	0.00	3A4
ATOM	1759	NE	ARG	267	56.515	2.666	11.644	1.00	0.00	3A4
MOTA	1760	CZ	ARG	267	55.718	2.342	12.715	1.00	0.00	3A4
ATOM	1761		ARG	267	55.829	1.104	13.280	1.00	0.00	3A4
MOTA	1762		ARG	267	54.819	3.229	13.235	1.00	0.00	3A4
ATOM	1763	С	ARG	267	55.443	7.575	12.488	1.00	0.00	3A4
ATOM	1764	0	ARG	267	55.403	8.776	12.757	1.00	0.00	3A4
ATOM	1765	N	VAL	268	55.180	6.600	13.409	1.00	0.00	3A4 3A4
ATOM	1766	CA	VAL	268 268	54.850 55.608	6.700 7.738	14.830 15.672	1.00	0.00	3A4
ATOM ATOM	1767 1768	CB	VAL	268	55.286	7.564	17.181	1.00	0.00	3A4
ATOM	1769		VAL	268	57.124	7.555	15.459	1.00	0.00	3A4
ATOM	1770	c	VAL	268	53.347	6.859	14.949	1.00	0.00	3A4
ATOM	1771	ŏ	VAL	268	52.814	7.966	14.876	1.00	0.00	3A4
ATOM	1772	N	ASP	269	52.650	5.703	15.128	1.00	0.00	3A4
ATOM	1773	CA	ASP	269	51.217	5.484	15.039	1.00	0.00	3A4
ATOM	1774	CB	ASP	269	50.952	4.008	14.629	1.00	0.00	3A4
MOTA	1775	CG	ASP	269	51.584	2.963	15.562	1.00	0.00	3A4
MOTA	1776		ASP	269	52.585	2.329	15.136	1.00	0.00	3A4
MOTA	1777		ASP	269	51.040	2.734	16.671	1.00	0.00	3A4
MOTA	1778	С	ASP	269	50.513	5.855	16.322	1.00	0.00	3A4
ATOM	1779	0	ASP	269	51.163	6.144	17.324	1.00	0.00	3A4 3A4
ATOM	1780	N	PHE	270	49.161	5.834	16.331	1.00	0.00	3A4
MOTA	1781	CA	PHE	270	48.362 46.855	6.204 6.258	17.490 17.148	1.00	0.00	3A4
ATOM ATOM	1782 1783	CB CG	PHE	270 270	45.990	6.766	18.282	1.00	0.00	3A4
ATOM	1784		PHE	270	45.280	5.854	19.081	1.00	0.00	3A4
ATOM	1785		PHE	270	46.020	8.114	18.661	1.00	0.00	3A4
ATOM	1786		PHE	270	44.531	6.282	20.177	1.00	0.00	3A4
ATOM	1787		PHE	270	45.309	8.546	19.789	1.00	0.00	3A4
ATOM	1788	CZ	PHE	270	44.542	7.634	20.522	1.00	0.00	3A4
ATOM	1789	С	PHE	270	48.565	5.305	18.696	1.00	0.00	3A4
ATOM	1790	0	PHE	270	48.623	5.789	19.822	1.00	0.00	3A4
MOTA	1791	N	LEU	271	48.707	3.980	18.488	1.00	0.00	3A4
ATOM	1792	CA	LEU	271	48.911	3.039	19.569	1.00	0.00	3A4
ATOM	1793	CB	LEU	271	48.798	1.584	19.058	1.00	0.00	3A4
ATOM	1794	CG	LEU	271	47.377	1.034	18.852	1.00	0.00	3A4 3A4
ATOM	1795		LEU	271	47.422 46.550	-0.399 1.035	18.277 20.150	1.00	0.00	3A4
ATOM ATOM	1796 1797	C	LEU	271 271	50.247	3.247	20.130	1.00	0.00	3A4
ATOM	1798	0	LEU	271	50.309	3.283	21.510	1.00	0.00	3A4
ATOM	1799	N	GLN	272	51.325	3.513	19.518	1.00	0.00	3A4
ATOM	1800	CA	GLN	272	52.641	3.856	20.018	1.00	0.00	3A4
ATOM	1801	СВ	GLN	272	53.651	3.973	18.871	1.00	0.00	3A4
ATOM	1802	CG	GLN	272	53.989	2.568	18.334	1.00	0.00	3A4
MOTA	1803	CD	GLN	272	54.908	2.656	17.119	1.00	0.00	3A4
ATOM	1804		GLN	272	55.225	3.735	16.626		0.00	3A4
ATOM	1805		GLN	272	55.347	1.475	16.611	1.00	0.00	3A4
ATOM	1806	C	GLN	272	52.646	5.136	20.813	1.00	0.00	3A4
ATOM	1807	0	GLN	272	53.254	5.214	21.874	1.00	0.00	3A4
ATOM	1808	N	LEU	273	51.883	6.155	20.356 21.048	1.00	0.00	3A4 3A4
MOTA MOTA	1809 1810	CA CB	LEU	273 273	51.695 50.926	7.415 8.433	20.166	1.00	0.00	3A4
ATOM	1811	CG	LEU	273	51.785	8.888	18.948	1.00	0.00	3A4
ATOM	1812		LEU	273	50.959	9.439	17.771	1.00	0.00	3A4
ATOM	1813		LEU	273	52.899	9.882	19.332	1.00	0.00	3A4
ATOM	1814	C	LEU	273	50.983	7.274	22.346	1.00	0.00	3A4
ATOM	1815	0	LEU	273	51.365	7.895	23.329	1.00	0.00	3A4
ATOM	1816	N	MET	274	49.964	6.395	22.412	1.00	0.00	3A4
MOTA	1817	CA	MET	274	49.244	6.073	23.621	1.00	0.00	3A4
MOTA	1818	СВ	MET	274	47.977	5.254	23.316	1.00	0.00	3A4
ATOM	1819	CG	MET	274	46.828	6.090	22.751	1.00	0.00	3A4
MOTA	1820	SD	MET	274	45.317	6.067	23.770	1.00	0.00	3A4
ATOM	1821	CE	MET	274	45.991	6.940	25.218	1.00	0.00	3A4 3A4
ATOM	1822	C	MET	274	50.109 50.038	5.325 5.567	24.619 25.819	1.00	0.00	3A4
ATOM ATOM	1823 1824	0 N	MET	274 275	50.038	4.417	24.131	1.00	0.00	3A4
ATOM	1825	CA	ILE	275 275	51.851	3.564	24.131	1.00	0.00	3A4
MOTA	1826	CB	ILE	275	52.467	2.441	24.078	1.00	0.00	3A4
ATOM	1827		ILE	275	53.965	2.545	23.648	1.00	0.00	3A4
ATOM	1828		ILE	275	52.209	1.038	24.643	1.00	0.00	3A4
ATOM	1829	CD	ILE	275	51.787	0.081	23.536	1.00	0.00	3A4

ATOM	1830	С	ILE	275	52.925	4.329	25.660	1.00	0.00		3A4
ATOM	1831	ŏ	ILE	275	53.323	3.975	26.764	1.00	0.00		3A4
ATOM	1832	N	ASP	276	53.392	5.425	25.033	1.00	0.00		3A4
ATOM	1833	CA	ASP	276	54.488	6.233	25.491	1.00	0.00		3A4
ATOM	1834	СВ	ASP	276	55.375	6.635	24.263	1.00	0.00		3A4
ATOM	1835	CG	ASP	276	56.766	7.177	24.648	1.00	0.00		3A4
ATOM	1836	OD1		276	57.527	6.432	25.323	1.00	0.00		3A4
ATOM	1837	OD2		276	57.080	8.336	24.266	1.00	0.00		3A4
ATOM	1838	C	ASP	276	53.994	7.467	26.229	1.00	0.00		3A4
ATOM	1839	ŏ	ASP	276	54.738	8.023	27.029	1.00	0.00		3A4
MOTA	1840	N	SER	277	52.734	7.918	25.959	1.00	0.00		3A4
ATOM	1841	CA	SER	277	51.962	9.005	26.574	1.00	0.00		3A4
ATOM	1842	СВ	SER	277	51.494	8.689	28.034	1.00	0.00		3A4
ATOM	1843	OG	SER	277	52.536	8.498	28.989	1.00	0.00		3A4
ATOM	1844	C	SER	277	52.586	10.401	26.477	1.00	0.00		3A4
MOTA	1845	ŏ	SER	277	53.547	10.719	27.177	1.00	0.00		3A4
ATOM	1846	N	GLN	278	52.027	11.259	25.584	1.00	0.00		3A4
	1847	CA	GLN	278	52.576	12.557	25.230	1.00	0.00		3A4
ATOM	1848	CB	GLN	278	53.079	12.585	23.748	1.00	0.00		3A4
ATOM	1849	CG	GLN	278	52.289	11.752	22.708	1.00	0.00		3A4
ATOM	1850	CD	GLN	278	50.896	12.317	22.436	1.00	0.00		3A4
ATOM		OE1		278	49.896	11.703	22.807	1.00	0.00		3A4
ATOM	1851	NE2		278	50.821	13.500	21,767	1.00	0.00		3A4
MOTA	1852			278	51.568	13.647	25.534	1.00	0.00		3A4
MOTA	1853 1854	C	GLN	278	51.306	14.524	24.712	1.00	0.00		3A4
MOTA		0	GLN	278	51.016	13.632	26.775	1.00	0.00		3A4
ATOM	1855	N	ASN		50.193	14.697	27.310	1.00	0.00		3A4
ATOM	1856	CA	ASN	279 279	48.716	14.690	26.781	1.00	0.00		3A4
ATOM	1857	CB	ASN	279	47.973	15.999	27.107	1.00	0.00		3A4
ATOM	1858	CG	ASN		47.305	16.089	28.136	1.00	0.00		3A4
ATOM	1859		ASN	279	48.086	17.026	26.221	1.00	0.00		3A4
ATOM	1860		ASN	279	50.239	14.505	28.808	1.00	0.00		3A4
MOTA	1861	C	ASN	279	50.626	15.409	29.546	1.00	0.00		3A4
MOTA	1862	0	ASN	279	49.821	13.405	29.277	1.00	0.00		3A4
ATOM	1863	N	SER	280		12.901	30.674	1.00	0.00		3A4
ATOM	1864	CA	SER	280	49.736	12.330	31.056	1.00	0.00		3A4
MOTA	1865	CB	SER	280	48.334 47.313	13.268	30.740	1.00	0.00		3A4
ATOM	1866	OG	SER	280		11.870	30.740	1.00	0.00		3A4
ATOM	1867	C	SER	280	50.810	11.569	30.079	1.00	0.00		3A4
ATOM	1868	0	SER	280	51.635	11.317	32.183	1.00	0.00		3A4
ATOM	1869	N	LYS	281	50.813	10.412	32.724	1.00	0.00		3A4
ATOM	1870	CA	LYS	281	51.810 52.318	10.412	34.135	1.00	0.00		3A4
MOTA	1871	CB	LYS	281		10.740	35.357	1.00	0.00		3A4
MOTA	1872	CG	LYS	281	51.368 50.099	11.612	35.328	1.00	0.00		3A4
MOTA	1873	CD	LYS	281 281	49.241	11.508	36.598	1.00	0.00		3A4
MOTA	1874	CE	LYS	281	48.695	10.139	36.770	1.00	0.00		3A4
ATOM	1875	NZ	LYS	281	51.259	9.009	32.800	1.00	0.00		3A4
MOTA	1876	C	LYS	281	50.051	8.792	32.725	1.00	0.00		3A4
ATOM	1877 1878	N O	GLU	282	52.179	8.025	33.003	1.00	0.00		3A4
ATOM		CA	GLU	282	51.902	6.623	33.252	1.00	0.00	•	3A4
ATOM	1879 1880	CB	GLU	282	52.839	5.684	32.439	1.00	0.00		3A4
ATOM	1881	CG	GLU	282	54.355	5.905	32.633	1.00	0.00		3A4
ATOM	1882	CD	GLU	282	55.125	5.055	31.617	1.00	0.00		3A4
ATOM	1883		GLU	282	54.983	5.322	30.393	1.00	0.00		3A4
ATOM			GLU	282	55.866	4.133	32.049	1.00	0.00		3A4
ATOM ATOM	1884 1885	C	GLU	282	52.026	6.378	34.739	1.00	0.00		3A4
	1886	ò	GLU	282	52.842	7.002	35.416	1.00	0.00		3A4
ATOM ATOM	1887	И	THR	283	51.169	5.468	35.281	1.00	0.00		3A4
ATOM	1888	CA	THR	283	50.949	5.262	36.708	1.00	0.00		3A4
ATOM	1889	СВ	THR	283	49.462	5.076	37.037	1.00	0.00		3A4
ATOM	1890		THR	283	48.843	4.071	36.236	1.00	0.00		3A4
ATOM	1891		THR	283	48.746	6.425	36.797	1.00	0.00		3A4
MOTA	1892	C	THR	283	51.786	4.117	37.266	1.00	0.00		3A4
ATOM	1893	ŏ	THR	283	51.843	3.935	38.481	1.00	0.00		3A4
ATOM	1894	N	GLU	284	52.457	3.329	36.385	1.00	0.00		3A4
ATOM	1895	CA	GLU	284	53.336	2.253	36.792	1.00	0.00		3A4
ATOM	1896	CB	GLU	284	52.583	0.907	37.025	1.00	0.00		3A4
MOTA	1897	CG	GLU	284	53.427	-0.211	37.670	1.00	0.00		3A4
ATOM	1898	CD	GLU	284	52.553	-1.452	37.873	1.00	0.00		3A4
MOTA	1899		GLU	284	52.075	-2.014	36.851	1.00	0.00		3A4
MOTA	1900		GLU	284	52.352	-1.855	39.051	1.00	0.00		3A4
MOTA	1901	C	GLU	284	54.393	2.152	35.719	1.00	0.00		3A4
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MOTA	1902	0	GLU	284	55.397	2.861	35.770	1.00	0.00	3A4
ATOM	1903	N	SER	285	54.186	1.256	34.721	1.00	0.00	3A4
ATOM	1904	CA	SER	285	55.139	0.973	33.669	1.00	0.00	3A4
MOTA	1905	CB	SER	285	56.281	-0.008	34.108	1.00	0.00	3A4
ATOM	1906	OG	SER	285	55.800	-1.171	34.781	1.00	0.00	3A4
ATOM	1907	C	SER	285	54.331 54.522	0.438	32.510 32.066	1.00	0.00	3A4 3A4
ATOM	1908	0	SER	285	53.396	-0.694 1.275	31.998	1.00	0.00	3A4
MOTA MOTA	1909 1910	N Ca	HIS HIS	286 286	52.522	0.926	30.901	1.00	0.00	3A4
ATOM	1911		HIS	286	49.824	1.672	32.816	1.00	0.00	3A4.
ATOM	1912	CG	HIS	286	50.594	0.542	32.645	1.00	0.00	3A4
ATOM	1913	СВ	HIS	286	51.264	0.113	31.356	1.00	0.00	3A4
ATOM	1914	NE2	HIS	286	49.782	0.592	34.753	1.00	0.00	3A4
ATOM	1915	CD2	HIS	286	50.557	-0.106	33.843	1.00	0.00	3A4
MOTA	1916		HIS	286	49.366	1.652	34.090	1.00	0.00	3A4
ATOM	1917	C	HIS	286	52.192	2.222	30.200	1.00	0.00	3A4
MOTA	1918	0	HIS	286	53.089	2.937	29.758	1.00	0.00	3A4
ATOM	1919	N	LYS	287	50.878	2.537	30.069	1.00	0.00	3A4 3A4
ATOM	1920 1921	CA CB	LYS LYS	287 287	50.317 49.136	3.652 3.180	29.338 28.453	1.00	0.00	3A4
ATOM ATOM	1922	CG	LYS	287	49.553	2.209	27.349	1.00	0.00	3A4
ATOM	1923	CD	LYS	287	48.717	2.529	26.095	1.00	0.00	3A4
ATOM	1924	CE	LYS	287	48.931	1.795	24.736	1.00	0.00	3A4
ATOM	1925	NZ	LYS	287	47.885	2.079	23.732	1.00	0.00	3A4
ATOM	1926	С	LYS	287	49.794	4.698	30.287	1.00	0.00	3A4
MOTA	1927	0	LYS	287	49.872	4.548	31.504	1.00	0.00	3A4
ATOM	1928	N	ALA	288	49.185	5.771	29.701	1.00	0.00	3A4
ATOM	1929	CA	ALA	288	48.374	6.783	30.350	1.00	0.00	3A4
ATOM	1930	СВ	ALA	288	48.615	8.202	29.810	1.00	0.00	3A4
ATOM	1931	C	ALA	288 288	46.906 46.333	6.403 6.618	30.192 29.125	1.00	0.00	3A4 3A4
ATOM ATOM	1932 1933	о и	ALA LEU	289	46.245	5.810	31.226	1.00	0.00	3A4
ATOM	1934	CA	LEU	289	46.774	5.489	32.535	1.00	0.00	3A4
ATOM	1935	СВ	LEU	289	46.349	6.484	33.668	1.00	0.00	3A4
ATOM	1936	CG	LEU	289	44.839	6.740	33.920	1.00	0.00	3A4
ATOM	1937	CD1	LEU	289	44.604	7.179	35.378	1.00	0.00	3A4
ATOM	1938		LEU	289	44.221	7.776	32.951	1.00	0.00	3A4.
ATOM	1939	С	LEU	289	46.475	4.056	32.878	1.00	0.00	3A4
ATOM	1940	0	LEU	289	46.614	3.704	34.048	1.00	0.00	3A4
ATOM	1941 1942	N CA	SER	290 290	46.131 46.112	3.176 1.765	31.880 32.148	1.00	0.00	3A4 3A4
ATOM ATOM	1942		SER	290 ·	45.026	1.325	33.179	1.00	0.00	3A4·
ATOM	1944	OG .	SER	290	43.728	1.835	32.895	1.00	0.00	3A4
ATOM	1945	c	SER	290	45.931	1.008	30.867	1.00	0.00	3A4
ATOM	1946	0	SER	290	45.432	1.483	29.847	1.00	0.00	3A4
MOTA	1947	N	ASP	291	46.293	-0.287	30.944	1.00	0.00	3A4
MOTA	1948	CA	ASP	291	46.226	-1.223	29.856	1.00	0.00	3A4
MOTA	1949	СВ	ASP	291	46.894	-2.555	30.218	1.00	0.00	3A4
ATOM	1950	CG	ASP	291	48.385	-2.331	30.513	1.00	0.00	3A4
ATOM ATOM	1951 1952	OD1	ASP	291 291	49.127 48.800	-1.982 -2.508	29.555 31.690	1.00 1.00	0.00	3A4 3A4
ATOM	1953	C	ASP	291	44.820	-1.495	29.390	1.00	0.00	3A4
ATOM	1954	ŏ	ASP	291	44.578	-1.735	28.227	1.00	0.00	3A4
ATOM	1955	N	LEU	292	43.831				0.00	3A4
ATOM	1956	CA	LEU	292	42.433	-1.624	29.999	1.00	0.00	3A4
ATOM	1957	CB	LEU	292	41.659	-1.848	31.312	1.00	0.00	3A4
ATOM	1958	CG	LEU	292	41.910	-3.218	31.978	1.00	0.00	3A4
MOTA	1959	CD1		292	41.502	-3.197	33.463	1.00	0.00	3A4
ATOM	1960	CD2		292	41.193	-4.362	31.230	1.00	0.00	3A4
ATOM	1961	C	LEU	292	41.827	-0.445	29.268	1.00	0.00	3A4
MOTA	1962	0	LEU	292 293	41.078 42.216	-0.602 0.784	28.309 29.669	1.00	0.00	3A4 3A4
ATOM ATOM	1963 1964	N CA	GT0 GT0	293	42.216	2.025	29.064	1.00	0.00	3A4 3A4
ATOM	1965	CB	GLU	293	42.258	3.233	29.892	1.00	0.00	3A4
ATOM	1966	CG	GLU	293	41.403	3.396	31.163	1.00	0.00	3A4
ATOM	1967	CD	GLU	293	41.950	4.520	32.046	1.00	0.00	3A4
ATOM	1968	OE1		293	41.285	4.842	33.067	1.00	0.00	3A4
MOTA	1969	OE2	GLU	293	43.037	5.066	31.722	1.00	0.00	3A4
MOTA	1970	С	GLU	293	42.286	2.186	27.666	1.00	0.00	3A4
MOTA	1971	0	GLU	293	41.540	2.607	26.793	1.00	0.00	3A4
ATOM	1972	N	LEU	294	43.547	1.769	27.420	1.00	0.00	3A4
ATOM	1973	CA	LEU	294	44.175	1.802	26.122	1.00	0.00	3A4

ATOM	1974	СВ	LEU	294	45.633	1.380	26.208	1.00	0.00	3A4
ATOM	1975	CG	LEU	294	46.091	-0.086	26.051	1.00	0.00	3A4
ATOM	1976	CD1	LEU	294	46.203	-0.637	24.643	1.00	0.00	3A4
ATOM	1977	CD2	LEU	294 .	47.365	-0.436	26.810	1.00	0.00	3A4
ATOM	1978	С	LEU	294	43.443	0.944	25.134	1.00	0.00	3A4
MOTA	1979	0	LEU	294	43.172	1.361	24.020	1.00	0.00	3A4
MOTA	1980	N	VAL	295	43.044	-0.282	25.551	1.00	0.00	3A4 3A4
ATOM	1981	CA	VAL VAL	295 295	42.358 42.271	-1.242 -2.600	24.721 25.380	1.00	0.00	3A4
MOTA	1982 1983	CB	VAL	295	41.397	-3.622	24.599	1.00	0.00	3A4
MOTA MOTA	1984		VAL	295	43.701	-3.178	25.429	1.00	0.00	3A4
ATOM	1985	c	VAL	295	40.980	-0.762	24.357	1.00	0.00	3A4
ATOM	1986	ŏ	VAL	295	40.584	-0.846	23.207	1.00	0.00	3A4
ATOM	1987	N	ALA	296	40.252	-0.146	25.306	1.00	0.00	3A4
MOTA	1988	CA	ALA	296	38.945	0.439	25.074	1.00	0.00	3A4
ATOM	1989	CB	ALA	296	38.344	0.902	26.408	1.00	0.00	3A4
ATOM	1990	С	ALA	296	38.944	1.619	24.132	1.00	0.00	3A4
MOTA	1991	0	ALA	296	38.032	1.797	23.342	1.00	0.00	3A4 3A4
ATOM	1992 1993	N CA	GLN GLN	297 297	40.018 40.228	2.430 3.546	24.170 23.284	1.00	0.00	3A4
MOTA MOTA	1994	СВ	GLN	297	41.379	4.436	23.773	1.00	0.00	3A4
ATOM	1995	CG	GLN	297	40.914	5.233	25.008	1.00	0.00	3A4
ATOM	1996	CD	GLN	297	42.099	5.887	25.715	1.00	0.00	3A4
ATOM .	1997	OE1		297	43.052	5.222	26.114	1.00	0.00	3A4
MOTA	1998	NE2	GLN	297	42.034	7.228	25.902	1.00	0.00	3A4
MOTA	1999	С	GLN	297	40.505	3.108	21.882	1.00	0.00	3A4
MOTA	2000	0	GLN	297	39.872	3.572	20.943	1.00	0.00	3A4
MOTA	2001	N	SER	298	41.403	2.117	21.715	1.00	0.00	3A4 3A4
MOTA	2002 2003	CA	SER	298 298	41.744 42.925	1.546 0.563	20.434 20.529	1.00	0.00	3A4
ATOM ATOM	2003	CB OG	SER SER	298	42.771	-0.519	21.435	1.00	0.00	3A4
ATOM	2005	č	SER	298	40.584	0.872	19.755	1.00	0.00	3A4
ATOM	2006	ō	SER	298	40.435	0.977	18.546	1.00	0.00	3A4
ATOM	2007	N	ILE	299	39.688	0.228	20.542	1.00	0.00	3A4
MOTA	2008	ÇA	ILE	299	38.438	-0.363	20.098	1.00	0.00	3A4
MOTA	2009	СВ	ILE	299	37.670	-1.032	21.291	1.00	0.00	3A4
MOTA	2010		ILE	299	36.134	-1.268	21.098	1.00	0.00	3A4
ATOM	2011	CG1	ILE	299	38.328	-2.333	21.803	1.00	0.00	3A4 3A4
ATOM ATOM	2012 2013	CD	ILE	299 299	37.787 37.515	-3.619 0.677	21.185 19.534	1.00	0.00	3A4
ATOM	2013	Ö	ILE	299	36.949	0.525	18.457	1.00	0.00	3A4
ATOM	2015	N	ILE	300	37.374	1.799	20.268	1.00	0.00	3A4
ATOM	2016	CA	ILE	300	36.494		19.921	1.00	0.00	3A4
ATOM	2017	СВ	ILE	300	36.290	3.798	21.113	1.00	0.00	3A4
ATOM	2018		ILE	300	36.292	5.340	20.897	1.00		3A4
MOTA	2019		ILE	300	34.906	3.296	21.637	1.00	0.00	3A4
MOTA	2020	CD	ILE	300	34.503	3.642	23.050	1.00	0.00	3A4 3A4
MOTA MOTA	2021 2022	С О	ILE	300 300	36.962 36.161	3.618 3.994	18.712 17.872	1.00	0.00	3A4
ATOM	2023	N	PHE	301	38.279	3.774	18.515	1.00	0.00	3A4
ATOM	2024	CA	PHE	301	38.819	4.525	17.406	1.00	0.00	3A4
ATOM	2025	СВ	PHE	301	40.332	4.745	17.663	1.00	0.00	3A4
ATOM	2026	CG	PHE	301	40.520	5.958	18.535	1.00	0.00	3A4
MOTA	2027		PHE	301	41.157	5.931	19.784	1.00	0.00	3A4
ATOM	2028		PHE	301	39.913	7.144	18.106	1.00	0.00	3A4
MOTA	2029		PHE	301	41.032	7.015	20.660	1.00	0.00	3A4 3A4
ATOM ATOM	2030 2031	CE2	PHE	301 301	39.784 40.300	8.213 8.142	18.969 20.259	1.00	0.00	3A4
ATOM	2032	C	PHE	301	38.633	3.743	16.111	1.00	0.00	3A4
ATOM	2033	ŏ	PHE	301	38.332	4.306	15.062	1.00	0.00	3A4
ATOM	2034	N	ILE	302	38.742	2.401	16.178	1.00	0.00	3A4
ATOM	2035	CA	ILE	302	38.511	1.491	15.076	1.00	0.00	3A4
MOTA	2036	СВ	ILE	302	39.005	0.104	15.470	1.00	0.00	3A4
MOTA	2037		ILE	302	38.482	-1.056	14.570	1.00	0.00	3A4
ATOM	2038		ILE	302	40.563	0.105	15.527	1.00	0.00	3A4
ATOM	2039	CD	ILE	302	41.293	0.195	14.178	1.00	0.00	3A4 3A4
MOTA MOTA	2040 2041	С 0	ILE	302 302	37.054 36.732	1.462 1.682	14.656 13.491	1.00	0.00	3A4
ATOM	2041	N	PHE	302	36.732	1.231	15.610	1.00	0.00	3A4
ATOM	2042	CA	PHE	303	34.711	1.090	15.324	1.00	0.00	3A4
ATOM	2044	СВ	PHE	303	34.008	0.159	16.395	1.00	0.00	3A4
ATOM	2045	ÇG	PHE	303	33.072	0.735	17.449	1.00	0.00	3A4

MOTA	2046	CD1	PHE	303	31.783	1.209	17.127	1.00	0.00	3A4
ATOM	2047	CD2		303	33.443	0.706	18.808	1.00	0.00	3A4
MOTA	2048	CE1	PHE	303	30.911	1.674	18.121	1.00	0.00	3A4
MOTA	2049	CE2	PHE	303	32.572	1.155	19.810	1.00	0.00	3A4
ATOM	2050	CZ,	PHE	303	31.307	1.647	19.465	1.00	0.00	3A4 3A4
MOTA	2051	С	PHE	303	34.016	2.407	14.993	1.00	0.00	3A4 3A4
ATOM	2052	0	PHE	303	33.183	2.472	14.092 15.679	1.00	0.00	3A4
ATOM	2053	N	ALA	304	34.391 33.814	3.513 4.831	15.484	1.00	0.00	3A4
ATOM	2054	CA	ALA	304 304	34.124	5.826	16.638	1.00	0.00	3A4
ATOM	2055 2056	CB C	ALA ALA	304	34.221	5.470	14.208	1.00	0.00	3A4
ATOM ATOM	2057	ō	ALA	304	33.449	6.196	13.589	1.00	0.00	3A4
ATOM	2058	N	GLY	305	35.466	5.191	13.787	1.00	0.00	3A4
MOTA	2059	CA	GLY	305	36.037	5.755	12.599	1.00	0.00	3A4
ATOM	2060	C	GLY	305	35.766	5.044	11.304	1.00	0.00	3A4
MOTA	2061	0	GLY	305	36.028	5.603	10.243	1.00	0.00	3A4
MOTA	2062	N	TYR	306	35.257	3.789	11.337	1.00	0.00	3A4
ATOM	2063	CA	TYR	306	35.125	2.982	10.139	1.00	0.00	3A4
ATOM ·	2064	СВ	TYR	306	35.531	1.484	10.389	1.00	0.00	3A4 3A4
ATOM	2065	CG	TYR	306	35.403	0.528	9.206 7.858	1.00	0.00	3A4
MOTA	2066		TYR	306 306	35.378 35.19 5	0.950 -0.835	9.469	1.00	0.00	3A4
ATOM ATOM	2067 2068		TYR TYR	306	35.009	0.064	6.843	1.00	0.00	3A4
ATOM	2069		TYR	306	34.885	-1.738	8.441	1.00	0.00	3A4
ATOM	2070	CZ	TYR	306	34.766	-1.281	7.125	1.00	0.00	3A4
ATOM	2071	ОН	TYR	306	34.383	-2.159	6.089	1.00	0.00	3A4
ATOM	2072	C	TYR	306	33.741	3.132	9.572	1.00	0.00	3A4
ATOM	2073	0	TYR	306	33.566	3.553	8.431	1.00	0.00	3A4
ATOM	2074	N	GLU	307	32.692	2.781	10.344	1.00	0.00	3A4
ATOM	2075	CA	GLU	307	31.384	2.639	9.745	1.00	0.00	3A4
MOTA	2076	CB	GLU	307	30.517	1.553	10.437	1.00	0.00	3A4
MOTA	2077	CG	GLU	307	31.119	0.127	10.329	1.00	0.00	3A4 3A4
ATOM	2078	CD	GLU	307	31.130	-0.460 0.159	8.905 7.942	1.00	0.00	3A4
ATOM	2079		GLU	307 307	30.600 31.670	-1.592	8.778	1.00	0.00	3A4
ATOM ATOM	2080 2081	C	GLU	307	30.630	3.933	9.563	1.00	0.00	3A4
ATOM	2082	ŏ	GLU	307	29.605	3.926	8.924	1.00	0.00	· 3A4
ATOM	2083	N	THR	308	31.140	5.089	10.026	1.00	0.00	3A4
ΛΤΟM	2084	CA	THR	308	30.556	6.394	9.788	1.00	0.00	3A4
ATOM	2085	CB	THR	308	30.866	7.363	10.932	1.00	0.00	3A4
ATOM	2086	OG1	THR	308	32.255	7.423	11.254	1.00	0.00	3A4
ATOM	2087		THR	308	30.088	6.935	12.191	1.00	0.00	3A4 3A4
MOTA	2088	С	THR	308	31.006	6.957	8.463	1.00	0.00	3A4
ATOM	2089	0	THR	308	30.202	7.360	7.632 8.226	1.00	0.00	3A4
ATOM	2090	N	THR	309 309	32.332 32.979	6.929 7.436	7.038	1.00	0.00	3A4
ATOM	2091 2092	CA CB	THR THR	309	34.479	7.445	7.204	1.00	0.00	3A4
ATOM ATOM	2092		THR	309	34.937	6.213	7.743	1.00	0.00	3A4
ATOM	2094		THR	309	34.867	8.555	8.200	1.00	0.00	3A4
ATOM	2095	Ç	THR	309	32,600	6.684	5.779	1.00	0.00	3A4
ATOM	2096	0	THR	309	32.349	7.278	4.741	1.00	0.00	3A4
MOTA	2097	N	SER	310	32.484	5.339	5.875	1.00	0.00	3A4
MOTA	2098	CA	SER	310	32.052	4.458	4.809	1.00	0.00	3A4
ATOM	2099	CB	SER	310	31.996	2.990	5.310	1.00	0.00	3A4 3A4
MOTA	2100	OG	SER	310	33.306	2.563 4.763	5.646 4.322	1.00	0.00	3A4
MOTA	2101	C	SER	310	30.666 30.413	4.886	3.131	1.00	0.00	3A4
MOTA	2102	О И	SER SER	310 311	29.728	4.960	5.261	1.00	0.00	3A4
MOTA MOTA	2103 2104	CA	SER	311	28.351	5.245	4.950	1.00	0.00	3A4
ATOM	2105	СВ	SER	311	27.509	5.056	6.222	1.00	0.00	3A4
ATOM	2106	ŌĞ	SER	311	27.701	3.739	6.719	1.00	0.00	3A4
ATOM	2107	C	SER	311	28.153	6.627	4.389	1.00	0.00	3A4
ATOM	2108	0	SER	311	27.316	6.833	3.523	1.00	0.00	3A4
ATOM	2109	N	VAL	312	28.984	7.609	4.813	1.00	0.00	3A4
ATOM	2110	ÇA	VAL	312	28.964	8.970	4.310	1.00	0.00	3A4
MOTA	2111	СВ	VAL	312	29.781	9.902	5.173	1.00	0.00	3A4 3A4
ATOM	2112		VAL	312	29.980	11.315	4.570	1.00	0.00	3A4 3A4
ATOM	2113		VAL	312	28.894 29.408	10.077 9.072	6.433 2.884	1.00	0.00	3A4
ATOM	2114 2115	С 0	VAL VAL	312 312	28.751	9.739	2.103	1.00	0.00	3A4
MOTA MOTA	2115	N	LEU	312	30.463	8.328	2.495	1.00	0.00	3A4
ATOM	2117	CA	LEU	313	30.996	8.277	1.150	1.00	0.00	3A4
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ATOM	2118	СВ	LEU	313	32.294	7.466	1.085	1.00	0.00	3A4
ATOM	2119	CG	LEU	313	33.512	8.219	1.649	1.00	0.00	3A4
ATOM	2120	CD1	LEU	313	34.492	8.511	0.499	1.00	0.00	3A4
ATOM	2121	CD2	LEU	313	33.322	9.485	2.496	1.00	0.00	3A4
MOTA	2122	С	LEU	313	30.017	7.696	0.167	1.00	0.00	3A4
MOTA	2123	0	LEU	313	29.808	8.229	-0.917	1.00	0.00	3A4
ATOM	2124	N	SER	314	29.309	6.624	0.579	1.00	0.00	3A4
MOTA	2125	CA	SER	314	28.305	5.981	-0.243	1.00	0.00	3A4
ATOM	2126	CB	SER	314	27.992	4.570	0.299	1.00	0.00	3A4
MOTA	2127	OG	SER	314	29.195	3.821	0.397	1.00	0.00	3A4
ATOM	2128	С	SER	314	27.070	6.845	-0.420	1.00	0.00	3A4
ATOM	2129	0	SER	314	26.505	6.909	-1.507	1.00	0.00	3A4
ATOM	2130	N	PHE	315	26.702	7.636	0.625	1.00	0.00	3A4
ATOM	2131	CA	PHE	315	25.595	8.572	0.583	1.00	0.00	3A4
ATOM	2132	СВ	PHE	315	25.181	9.076	2.015	1.00	0.00	3A4
MOTA	2133	CG	PHE	315	23.897	8.407	2.456	1.00	0.00	3A4
ATOM	2134	CD1	PHE	315	23.856	7.678	3.662	1.00	0.00	3A4
ATOM	2135	CD2	PHE	315	22.732	8.451	1.660	1.00	0.00	3A4
MOTA	2136	CE1	PHE	315	22.683	7.024	4.067	1.00	0.00	3A4
MOTA	2137	CE2	PHE	315	21.568	7.770	2.047	1.00	0.00	3A4
MOTA	2138	CZ	PHE	315	21.542	7.061	3.254	1.00	0.00	3A4
ATOM	2139	С	PHE	315	25.938	9.760	-0.291	1.00	0.00	3A4
ATOM	2140	0	PHE	315	25.075	10.250	-1.011	1.00	0.00	3A4
MOTA	2141	N	ILE	316	27.230	10.200	-0.328	1.00	0.00	3A4
ATOM	2142	CA	ILE	316	27.669	11.286	-1.202	1.00	0.00	3A4
MOTA	2143	СВ	ILE	316	29.119	11.864	-1.060	1.00	0.00	3A4
MOTA	2144		ILE	316	29.128	13.291	-1.688	1.00	0.00	3A4
ATOM	2145		ILE	316	29.687	11.833	0.371	1.00	0.00	3A4 3A4
ATOM	2146	CD	ILE	316	30.950	12.629	0.687	1.00	0.00	3A4
MOTA	2147	C	ILE	316	27.559	10.926	-2.666	1.00	0.00	3A4
ATOM	2148	0	ILE	316	27.111	11.726	-3.476	1.00	0.00	3A4
ATOM	2149	N	MET	317	27.919	9.671 9.137	-3.009 -4.351	1.00	0.00	3A4
ATOM	2150	CA	MET	317	27.868 28.640	7.803	-4.441	1.00	0.00	3A4
ATOM	2151	CB	MET	317		8.007	-4.191	1.00	0.00	3A4
ATOM	2152	CG	MET	317	30.148 31.027	6.548	-3.550	1.00	0.00	3A4
ATOM	2153	SD	MET	317	32.475	7.489	-2.987	1.00	0.00	3A4
ATOM	2154	CE	MET	317 317	26.449	8.978	-4.853	1.00	0.00	3A4
ATOM	2155	C	MET	317	26.139	9.327	-5.986	1.00	0.00	3A4
ATOM	2156 2157	N N	MET TYR	318	25.516	8.539	-3.981	1.00	0.00	3A4
ATOM ATOM	2158	CA	TYR	318	24.101	8.458	-4.293	1.00	0.00	3A4
ATOM	2159	СВ	TYR	318	23.333	7.794	-3.134	1.00	0.00	3A4
	2160	CG	TYR	318	21.822	7.683	-3.312	1.00	0.00	3A4
ATOM	2161		TYR	318	21.269	7.039	-4.436	1.00	0.00	3A4
ATOM	2162		TYR	318	. 20.950	8.269	-2.372	1.00	0.00	3A4
ATOM	2163		TYR	318	19.881	6.987	-4.624	1.00	0.00	3A4
ATOM	21.64		TYR	318	19.560	8.209	-2.548	1.00	0.00	3A4
ATOM	2165	CZ	TYR	318	19.024	7.566	-3.675	1.00	0.00	3A4
ATOM	2166	ОН	TYR	318	17.625	7.498	-3.855	1.00	0.00	. 3A4
ATOM	2167	C	TYR	318	23.501	9.814	-4.592	1.00	0.00	3A4
ATOM	2168	0	TYR	318	22.759	9.967	-5.553	1.00	0.00	3A4
MOTA	2169	N	GLU	319	23.864	10.847	-3.796	1.00	0.00	3A4
ATOM	2170	CA	GLU	319	23.389	12.203	-3.970	1.00	0.00	3A4
ATOM	2171	CB	GLU	319	23.703	13.127	-2.775		0.00	3A4
MOTA	2172	CG	GLU	319	22.849	12.760	-1.559	1.00	0.00	3A4
MOTA	2173	CD	GLU	319	23.038	13.838	-0.506	1.00	0.00	3A4
ATOM	2174	OE1	GLU	319	24.202	14.049	-0.085	1.00	0.00	3A4
MOTA	2175	OE2	GLU	319	22.027	14.476	-0.119	1.00	0.00	3A4
ATOM	2176	С	GLU	319	23.894	12.847	-5.231	1.00	0.00	3A4
MOTA	2177	0	GLU	319	23.132	13.474	-5.951	1.00	0.00	3A4
MOTA	2178	N	LEU	320	25.170	12.641	-5.595	1.00	0.00	3A4
HOTA	2179	CA	LEU	320	25.713	13.161	-6.828	1.00	0.00	3A4 3A4
MOTA	2180	СВ	LEU	320	27.239	13.059	-6.841	1.00	0.00	
MOTA	2181	CG	LEU	320	27.880	14.027	-5.843	1.00	0.00	3A4
ATOM	2182		LEU	320	29.380	13.757	-5.709	1.00	0.00	3A4 3A4
ATOM	2183		LEU	320	27.611	15.489	-6.192	1.00	0.00	3A4 3A4
ATOM	2184	С	LEU	320	25.160	12.475	-8.048	1.00	0.00	3A4
MOTA	2185	0	LEU	320	24.977	13.105	-9.083 -7.933	1.00	0.00	3A4
MOTA	2186	N	ALA	321	24.818	11.177	-7.933 -8.990	1.00	0.00	3A4
ATOM	2187	CA	ALA	321	24.215	10.397	-8.645	1.00	0.00	3A4
ATOM	2188	CB	ALA	321	24.217	8.897	-8.645 -9.259	1.00	0.00	3A4
ATOM	2189	С	ALA	321	22.802	10.861	-2.235	1.00	0.00	V.11

ATOM	2190	0	ALA	321	22.338	10.884	-10.397	1.00	0.00	3A4
ATOM	2191	N	THR	322	22.103	11.305	-8.194	1.00	0.00	3A4
ATOM	2192	CA	THR	322	20.743	11.780	-8.258	1.00	0.00	3A4
ATOM	2193	СВ	THR	322	19.981	11.519	-6.972	1.00	0.00	3A4
ATOM	2194	0G1		322	20.610	11.999	-5.794	1.00	0.00	3A4
ATOM	2195	CG2		322	19.745	9.994	-6.849	1.00	0.00	3A4
ATON	2196	c	THR	322	20.627	13.242	-8.642	1.00	0.00	3A4
	2197	o	THR	322	19.555	13.704	-9.018	1.00	0.00	3A4
ATOM		N	HIS	323	21.731	14.006	-8.558	1.00	0.00	3A4
MOTA	2198	CA	HIS	323	21.740	15.416	-8.856	1.00	0.00	3A4
ATOM	2199	ND1		323	20.544	15.212	-5.650	1.00	0.00	3A4
MOTA	2200		HIS	323	20.676	16.147	-6.653	1.00	0.00	3A4
MOTA	2201	CG		323	21.859	16.259	-7.581	1.00	0.00	3A4
ATOM	2202	CB	HIS	323	18.715	16.470	-5.582	1.00	0.00	3A4
MOTA	2203	NE2		323	19.549	16.908	-6.595	1.00	0.00	3A4
ATOM	2204	CD2			19.356	15.449	-5.043	1.00	0.00	3A4
MOTA	2205		HIS	323	22.892	15.711	-9.775	1.00	0.00	3A4
MOTA	2206	C	HIS	323		16.309	-9.352	1.00	0.00	3A4
ATOM	2207	0	HIS	323	23.883		-11.076	1.00	0.00	3A4
ATOM	2208	N	PRO	324	22.833		-12.002	1.00	0.00	3A4
MOTA	2209	CA	PRO	324	23.958			1.00	0.00	3A4
ATOM	2210	CD	PRO	324	21.602		-11.765	1.00	0.00	3A4
MOTA	2211	СB	PRO	324	23.420		-13.300	1.00	0.00	3A4
MOTA	2212	CG	PRO	324	21.905		-13.255		0.00	3A4
MOTA	2213	С	PRO	324	24.415		-12.213	1.00		3A4
MOTA	2214	0	PRO	324	25.575		-12.534	1.00	0.00	3A4
ATOM	2215	N	ASP	325	23.561		-11.949	1.00	0.00	
ATOM	2216	ÇA	ASP	325	23.917		-12.002	1.00	0.00	3A4 3A4
MOTA	2217	CB	ASP	325	22.668		-11.821	1.00	0.00	3A4
ATOM	2218	CG	ASP	325	21.653		-12.931	1.00	0.00	
MOTA	2219		ASP	325	21.991		-14.125	1.00	0.00	3A4 3A4
ATOM	2220		ASP	325	20.531		-12.600	1.00	0.00	3A4
MOTA	2221	С	ASP	325	24.927		-10.944	1.00	0.00	3A4
MOTA	2222	0	ASP	325	25.817		-11.169	1.00	0.00	
MOTA	2223	И	VAL	326	24.835	19.071	-9.767	1.00	0.00	3A4
ATOM	2224	CA	VAL	326	25.742	19.249	-8.647	1.00	0.00	3A4
ATOM	2225	·CB	VAL	326	25.198	18.672	-7.341	1.00	0.00	3A4
ATOM	2226	CG1	VAL	326	26.201	18.872	-6.173	1.00	0.00	3A4
ATOM	2227	CG2	VAL	326	23.874	19.402	-7.034	1.00	0.00	3A4
MOTA	2228	С	VAL	326	27.083	18.648	-8.960	1.00	0.00	3A4
MOTA	2229	0	VAL	326	28.106	19.288	-8.782	1.00	0.00	3A4
MOTA	2230	N	GLN	327	27.089	17.427	-9.528	1.00	0.00	3A4
MOTA	2231	CA	GLN	327	28.281	16.718	-9.931	1.00	0.00	3A4
MOTA	2232	CB	GLN	327	27.899		-10.487	1.00	0.00	3A4
MOTA	2233	CG	GLN	327	29.062		-10.683	1.00	0.00	3A4
ATOM	2234	CD	GLN	327	28.538		-11.166	1.00	0.00	3A4
MOTA	2235	OE1	GLN	327	27.336		-11.186	1.00	0.00	3A4
ATOM	2236	NE2	GLN	327	29.475		-11.572	1.00	0.00	3A4
ATOM	2237	С	GLN	327	29.088		-10.960	1.00	0.00	3A4
MOTA	2238	0	GLN	327	30.301		-10.855	1.00	0.00	3A4
ATOM	2239	N	GLN	328	28.408		-11.941	1.00	0.00	3A4
ATOM	2240	CA	GLN	328	29.023		-12.995	1.00	0.00	3A4
ATOM	2241	CB	GLN	328	27.97 7		-14.041	1.00	0.00	3A4
MOTA	2242	CG	GLN	328	27.544		-14.957	1.00	0.00	3A4
MOTA	2243	CD	GLN	328	26.423		-15.885	1.00	0.00	3A4
ATOM	2244	OE1	GLN	328	26.675		-16.800	1.00	0.00	3A4
MOTA	2245	NE2	GLN	328	25.164		-15.654	1.00	0.00	3A4
MOTA	2246	С	GLN	328	29.711		-12.470	1.00	0.00	3A4
ATOM	2247	0	GLN	328	30.827		-12.855	1.00	0.00	3A4
ATOM	2248	N	LYS	329	29.068		-11.501	1.00	0.00	3A4
ATOM	2249	CA	LYS	329	29.59 7		-10.807	1.00	0.00	3A4
ATOM	2250	СВ	LYS	329	28.515	22.465		1.00	0.00	3A4
MOTA	2251	CG	LYS	329	28.752	23.857		1.00	0.00	3A4
ATOM	2252	CD	LYS	329	27.533	24.347	_	1.00	0.00	3A4
ATOM	2253	CE	LYS	329	27.679	25.785		1.00	0.00	3A4
MOTA	2254	NZ	LYS	329	26.477	26.210		1.00	0.00	3A4
ATOM	2255	С	LYS	329	30.884		-10.052	1.00	0.00	3A4
MOTA	2256	0	LYS	329	31.860		-10.101	1.00	0.00	324
ATOM	2257	N	LEU	330	30.952	20.423		1.00	0.00	3A4
MOTA	2258	CA	LEU	330	32.100	19.968		1.00	0.00	3A4
ATOM	2259	СВ	LEU	330	31.814	18.742		1.00	0.00	3A4
MOTA	2260	CG	LEU	330	30.502	18.756		1.00	0.00	3A4
MOTA	2261	CĐ1	LEU	330	30.541	17.732	-5.920	1.00	0.00	3A4

N/DOM	2262	CD2	7 613	330	29.986	20.145 -6.584	1.00	0.00	3A4
MOTA							1.00	0.00	3A4
MOTA	2263	С	LEU	330	33.250	19.598 -9.579			
ATOM	2264	0	LEU	330	34.410	19.864 -9.296	1.00	0.00	3A4
	2265	N.	GLN	331	32.931	18.993 -10.741	1.00	0.00	3A4
MOTA							1.00	0.00	3A4
MOTA	2266	CA	GLN	331	33.881	18.627 -11.762			
ATOM	2267	CB	GLN	331	33.229	17.787 -12.880	1.00	0.00	3A4
		CG	GLN	331	32.942	16.354 -12.389	1.00	0.00	3A4
MOTA	2268								
ATOM	2269	CD	GLN	331	32.147	15.568 -13.437	1.00	0.00	3A4
MOTA	2270	OE1	GLN	331	31.063	15.988 -13.839	1.00	0.00	3A4
						14.396 -13.885	1.00	0.00	3A4
MOTA	2271	NE2		331	32.677	_			
ATOM	2272	С	GLN	331	34.500	19.817 -12.447	1.00	0.00	3A4
MOTA	2273	0	GLN	331	35.682	19.821 -12.771	1.00	0.00	3A4
				332	33.723	20.913 -12.594	1.00	0.00	3A4
ATOM	2274	N	GLU						
ATOM	2275	CA	GLU	332	34.188	22.185 -13.099	1.00	0.00	3A4
ATOM	2276	CB'	CLU	332	33.019	23.173 -13.413	1.00	0.00	3A4
				332	32.212	22.808 -14.675	1.00	0.00	3A4
ATOM ·	2277	CG	GLU						
ATOM	2278	CD	GLU	332	33.080	22.951 -15.931	1.00	0.00	3A4
ATOM	2279	OE1	GLU	332	33.533	24.092 -16.217	1.00	0.00	3A4
		OE2		332	33.301	21.919 -16.622	1.00	0.00	3A4
ATOM	2280								3A4
ATOM	2281	С	GLU	332	35.190	22.869 -12.182	1.00	0.00	
ATOM	2282	0	GLU	332	35.834	23.799 -12.629	1.00	0.00	3A4
	2283	N	GLU	333	35.484	22.350 -10.947	1.00	0.00	3A4
MOTA								0.00	3A4
ATOM	2284	CA	GLU	333	36.662	22.661 -10.132	1.00		
ATOM	2285	CB	GLU	333	36.449	22.284 -8.639	1.00	0.00	3A4
	2286	CG	GLU	333	35.228	22.936 -7.985	1.00	0.00	3A4
									3A4
ATOM	2287	CD	GLU	333	35.046	22.273 -6.620	1.00	0.00	
ATOM	2288	OE1	GLU	333	35.918	22.455 -5.730	1.00	0.00	3A4
ATOM	2289		GLU	333	34.038	21.540 -6.462	1.00	0.00	3A4
							1.00		3A4
ATOM	2290	С	GLU	333	37.923	21.912 -10.581		0.00	
ATOM	2291	0	GLU	333	38.425	21.038 -9.874	1.00	0.00	3A4
ATOM	2292	N	ILE	334	38.469	22.262 -11.773	1.00	0.00	3A4
								0.00	3A4
ATOM	2293.	CA	ILE	334	39.710	21.726 -12.300	1.00		
ATOM	2294	СВ	ILE	334	39.559	20.353 -12.973	1.00	0.00	3A4
ATOM	2295	CG2	ILE	334	38.582	20.368 -14.182	1.00	0.00	3A4
						19.687 -13.257	1.00	0.00	3A4
ATOM	2296	CG1	ILE	334	40.932				
ATOM	2297	CD	ILE	334	40.838	18.213 -13.660	1.00	0.00	3A4
ATOM	2298	С	ILE	334	40.231	22.836 -13.189	1.00	0.00	3A4
						22.658 -14.358	1.00	0.00	.3A4
ATOM	2299	0	ILE	334	40.570				
ATOM	2300	N	ASP	335	40.294	24.063 -12.600	1.00	0.00	3A4
ATOM	2301 -	CA	ASP	335	40.593	25.320 -13.260	1.00	0.00	3A4
				335	39.726	26.490 -12.699	1.00	0.00	3A4
ATOM	2302	CB	ASP						3A4
ATOM	2303	CG	ASP	335	38.240	26.203 -12.943	1.00	0.00	
ATOM	2304	OD1	ASP	335	37.854	26.015 -14.129	1.00	0.00	3A4
ATOM	2305	OD2		335	37.469	26.175 -11.947	1.00	0.00	3A4
									3A4
ATOM	2306	С	ASP	335	42.054	25.655 -13.079	1.00	0.00	
ATOM	2307	0	ASP	335	42.537	25.781 -11.956	1.00	0.00	3A4
ATOM	2308	N	ALA	336	42.772	25.816 -14.223	1.00	0.00	3A4
									3A4
MOTA	2309	CA	ALA	336	44.168	26.192 -14.316	1.00	0.00	
ATOM	2310	CB	ALA	336	45.027	25.116 -15.028	.1.00	0.00	3A4
ATOM	2311	С	ALA	336	44.207	27.500 -15.065	1.00	0.00	3A4
					44.428	27.544 -16.275	1.00	0.00	3A4
ATOM	2312	0	ALA	336					
ATOM	2313	N	VAL	337	43.963	28.609 -14.313	1.00	0.00	3A4
ATOM	2314	CA	VAL	337	43.815	29.978 -14.773	1.00	0.00	3A4
	2315	СВ	VAL	337	42.641	30.686 -14.085	1.00	0.00	3A4
MOTA									
ATOM	2316	CG1	VAL	337	42.436	32.130 -14.612	1.00	0.00	3A4
MOTA	2317	CG2	VAL	337	41.367	29.847 -14.326	1.00	0.00	3A4
ATOM	2318	C	VAL	337	45.115	30.696 -14.492	1.00	0.00	3A4
								0.00	3A4
ATOM	2319	0	VAL	337	45.661	30.605 -13.394	1.00		
ATOM	2320	N	LEU	338	45.621	31.439 -15.517	1.00	0.00	3A4
ATOM	2321	CA	LEU	338	46.821	32.257 -15.500	1.00	0.00	3A4
						32.088 -16.799		0.00	3A4
ATOM	2322	СВ	LEU	338	47.678				
ATOM	2323	CG	LEU	338	48.507	30.778 -16.897		0.00	3A4
ATOM	2324		LEU	338	47.680	29.494 -17.124	1.00	0.00	3A4
						30.909 -17.984	1.00	0.00	· 3A4
ATOM	2325		LEU	338	49.592				
ATOM	2326	С	LEU	338	46.355	33.705 -15.361	1.00	0.00	3A4
MOTA	2327	0	LEU	338	45.265	34.009 -15.844	1.00	0.00	3A4
					47.103	34.638 -14.719		0.00	3A4
ATOM	2328	N	PRO	339					
ATOM	2329	CA	PRO	339	46.612	35.949 -14.286		0.00	3A4
ATOM	2330	CD	PRO	339	48.443	34.363 ~14.196	1.00	0.00	3A4
	2331	СВ	PRO	339	47.610	36.376 -13.189		0.00	3A4
MOTA									3A4
MOTA	2332	CG	PRO	339	48.922	35.669 ~13.552		0.00	
ATOM	2333	C	PRO	339	46.561	36.955 -15.437	1.00	0.00	3A4

MOTA	2334	0	PRO	339	47.465	36.980	-16.272	1.00	0.00	3A4
ATOM	2335	N	ASN	340	45.491		-15.465	1.00	0.00	3A4
MOTA	2336	CA	ASN	340	45.246		-16.464	1.00	0.00	3A4 3A4
MOTA	2337	СВ	ASN	340	44.189		-17.523	1.00	0.00	3A4
ATOM	2338	CG	ASN	340 340	44.036 42.986		-18.704 -18.858	1.00	0.00	3A4
ATOM ATOM	2339 2340	OD1 ND2		340	45.094		-19.550	1.00	0.00	3A4
ATOM	2341	C	ASN	340	44.785		-15.672	1.00	0.00	3A4
ATOM	2342	0	ASN	340	45.452		-15.645	1.00	0.00	3A4
MOTA	2343	N	LYS	341	43.617		-14.997	1.00	0.00	3A4 3A4
ATOM	2344	CA	LYS	341 341	43.059 42.250		-14.095 -14.822	1.00	0.00	3A4
ATOM ATOM	2345 2346	CB CG	LYS LYS	341	41.892		-13.936	1.00	0.00	3A4
ATOM	2347	CD	LYS	341	41.220		-14.664	1.00	0.00	3A4
ATOM	2348	CE	LYS	341	39.708		-14.924	1.00	0.00	3A4
MOTA	2349	ΝZ	LYS	341	39.409		-15.994	1.00	0.00	3A4 3A4
ATOM	2350	C	LYS	341	42.197 40.991		-13.158 -13.036	1.00 1.00	0.00 0.00	3A4
ATOM ATOM	2351 2352	N N	LYS ALA	341 342	42.834		-12.482	1.00	0.00	3A4
ATOM	2353	CA	ALA	342	42.189		-11.577	1.00	0.00	3A4
ATOM	2354	CB	ALA	342	41.316		-12.306	1.00	0.00	3A4
MOTA	2355	С	ALA	342			-10.839	1.00 1.00	0.00	3A4 3A4
ATOM	2356	0	ALA PRO	342 343	44.413 43.106	36.880	-11.386 -9.614	1.00	0.00	3A4
ATOM ATOM	2357 2358	N CA	PRO	343	44.072	36.050	-8.891	1.00	0.00	3A4
ATOM	2359	CD	PRO	343	41.953	37.220	-8.779	1.00	0.00	3A4
ATOM	2360	CB	PRQ		43.605	36.121	-7.421	1.00	0.00	3A4
ATOM	2361	CG	PRO	343	42.097	36.392	-7.496	1.00	0.00 0.00	3A4 3A4
ATOM ATOM	2362 2363	С 0	PRO PRO	343 343	44.071 42.970	34.607 34.083	-9.441 -9.619	1.00	0.00	3A4
ATOM.	2364	N	PRO	344	45.209	33.930	-9.727	1.00	0.00	3A4
ATOM	2365	CA	PRO	344.	45.259		-10.448	1.00	0.00	3A4
MOTA	2366	CD	PRO	344.	- 46.542	34.509	-9.559	1.00	0.00	3A4
MOTA	2367	CB	PRO	344	46.678		-11.047 -10.077	1.00	0.00	3A4 3A4
MOTA .	2368 2369	.c	PRO PRO	344 344	47.532 45.002	31.473	-9.520	1.00	0.00	3A4
MOTA	2370	o	PRO	344	45.522	31.443	-8.404	1.00	0.00	3A4
ATOM	2371	N	THR	345	44.206		-10.004	1.00	0.00	3A4
ATOM	2372	CA	THR	345	43.860	29.247	-9.324	1.00	0.00	3A4 3A4
ATOM	2373 2374	CB	THR	345 345	42.343 41.981	29.124 27.994	-9.107 -8.315	1.00	0.00	3A4
ATOM ATOM	2375		THR	345	41.532		-10.430	1.00	0.00	3A4
ATOM	2376	С	THR	345	44.457	28.142	-10.173	1.00	0.00	3A4
ATOM	2377	0	THR	345	44.489		-11.397	1.00	0.00	3A4
ATOM	2378	N	TYR	346	44.964 45.601	27.063	-9.521 -10.173	1.00	0.00	3A4 3A4
ATOM ATOM	2379 2380	CA CB	TYR TYR	346 346	47.162		-10.173	1.00	0.00	3A4
ATOM	2381	CG	TYR	346	47.679		-10.925	1.00	0.00	3A4
ATOM	2382	CD1	ΤYR	346	48.250		-10.287	1.00	0.00	3A4
ATOM	2383		TYR	346	47.581		-12.331 -11.032	1.00	0.00	3A4 3A4
MOTA	2384 2385		TYR TYR	346 346	48.713 48.037		-13.082	1.00	0.00	3A4
MOTA MOTA	2386	CZ	TYR	346	48.606	29.335	-12.431	1.00	0.00	3A4
ATOM	2387	ОН	TYR	346	49.065		-13.178	1.00	0.00	3A4-
ATOM	2388	С	TYR	346	45.106	24.709		1.00	0.00	3A4 3A4
ATOM	2389	0	TYR	346	45.423 44.302	24.491	-8.285 -10.168	1.00	0.00	3A4
MOTA MOTA	2390 2391	N CA	ASP ASP	347 347	43.715	22.647		1.00	0.00	3A4
ATOM	2392	СВ	ASP	347	42.187	22.761		1.00	0.00	3A4
MOTA	2393	CG	ASP	347	41.948	23.760		1.00	0.00	3A4
ATOM	2394		ASP	347	41.329	24.825		1.00	0.00	3A4 3A4
ATOM ATOM	2395 2396	OD2 C	ASP ASP	347 347	42.386 43.937	23.474	-7.102 -10.781	1.00	0.00	3A4
ATOM	2397	Ö	ASP	347	43.549		-11.927	1.00	0.00	3A4
ATOM	2398	N	THR	348	44.581	20.493	-10.427	1.00	0.00	3A4
ATOM	2399	CA	THR	348	44.908		-11.314	1.00	0.00	3A4
ATOM	2400	CB	THR	348	46.416		-11.501 -12.006	1.00	0.00	3A4 3A4
MOTA MOTA	2401 2402		THR	348 348	46.987 46.725		-12.500	1.00	0.00	3A4
ATOM	2402	C	THR	348	44.258		-10.688	1.00	0.00	3A4
ATOM	2404	ŏ	THR	348	43.393		-11.293	1.00	0.00	3A4
ATOM	2405	N	VAL	349	44.670	17.854	-9.434	1.00	0.00	3A4

ATOM	2406	CA	VAL	349	44.059	16.848	-8.590	1.00	0.00		3A4
MOTA	2407	CB	VAL '	349	44.630	15.437	-8.788	1.00	0.00		3A4
MOTA	2408		VAL	349	46.169	15.347	-8.617	1.00	0.00		3A4
MOTA	2409		VAL	349	43.834	14.402	-7.958 -7.201	1.00	0.00		3A4 3A4
ATOM	2410	С 0	VAL VAL	349 349	44.175 44.934	17.435 16.990	-7.201 -6.341	1.00	0.00		3A4
ATOM ATOM	2411 2412	N	LEU	350	43.387	18.518	-6.988	1.00	0.00		3A4
MOTA	2413	CA	LEU	350	43.440	19.369	-5.824	1.00	0.00		3A4
ATOM	2414	СВ	LEU	350	44.479	20.520	-6.024	1.00	0.00		3A4
MOTA	2415	CG	LEU	350	44.847	21.374	-4.785	1.00	0.00		3A4
MOTA	2416		LEU	350	45.497	20.539	-3.662	1.00	0.00		3A4
MOTA	2417		LEU	350	45.743	22.560	-5.187	1.00	0.00		3A4
ATOM	2418	C	LEU	350	42.042	19.913	-5.672	1.00	0.00		3A4 3A4
ATOM	2419 2420	И .	.GLN	350 351	41.270 41.689	19.945 20.372	-6.631 -4.436	1.00	0.00		3A4
MOTA MOTA	2421	CA	GLN	351	40.404	20.942	-4.059	1.00	0.00		3A4
ATOM	2422	ÇB	GLN	351	40.005	20.645	-2.573	1.00	0.00		3A4
MOTA	2423	CG	GLN	351	40.814	21.289	-1.417	1.00	0.00		3A4
ATOM	2424	CD	GLN	351	42.269	20.816	-1.386	1.00	0.00		3A4
ATOM	2425		GLN	351	43.177	21.634	-1.520	1.00	0.00		3A4
ATOM	2426		GLN	351	42.505	19.487	-1.200	1.00	0.00		3A4 3A4
ATOM	2427 2428	С 0	GLN GLN	351 351	40.390 41.399	22.432 23.112	-4.305 -4.117	1.00	0.00		3A4
ATOM ATOM	2429	N	MET	352	39.214	22.962	-4.740	1.00	0.00		3A4
ATOM	2430	CA	MET	352	38.994	24.368	-5.014	1.00	0.00		3A4
ATOM	2431	СВ	MET	352	38.436	24.632	-6.438	1.00	0.00		3A4
MOTA	2432	CG	MET	352	38.472	26.097	-6.900	1.00	0.00		3A4
MOTA	2433	SD	MET	352	37.969	26.316	-8.633	1.00	0.00		3A4
MOTA	2434	CE	MET	352	38.075	28.129	-8.608	1.00	0.00		3A4
MOTA	2435	C	MET	352	38.113	24.911 25.287	-3.914 -2.866	1.00	0.00		3A4 3A4
ATOM ATOM	2436 2437	N	MET GLU	352 353	38.636 36.765	25.000	-4.117	1.00	0.00		3A4
ATOM	2438	CA	GLU	353	35.914	25.749	-3.211	1.00	0.00		3A4
ATOM	2439	CB	GLU	353	35.689	27.217	-3.688	1.00	0.00		3A4
ATOM	2440	CG	GLU	353	36.922	28.142	-3.627	1.00	0.00		3A4
ATOM	2441	CD	GLU	353	36.543	29.540	-4.126	1.00		•	3A4
ATOM	2442		GLU	353	36.622	30.504	-3.318	1.00	0.00		3A4 3A4
ATOM ATOM	2443 2444	C C	GLU	353 353	36.171 34.592	29.660 25.102	-5.325 -2.984	1.00	0.00		3A4
ATOM	2445	õ	GLU	353	34.078	25.104	-1.864	1.00	0.00		3A4
ATOM	2446	N	TYR	354	33.979	24.537	-4.047		0.00		3A4
MOTA	2447	CA	TYR	354	32.629	24.016	-3.996	1.00	0.00	•	3A4
MOTA	2448	CB	TYR	354	31.928	24.005	-5.369	1.00	0.00		3A4
ATOM	2449	CG	TYR	354	31.880	25.395	-5.954	1.00	0.00		3A4
ATOM	2450		TYR	354	32.962	25.916	-6.691 -5.783	1.00	0.00		3A4 3A4
ATOM ATOM	2451 2452		TYR TYR	354 354	30.740 32.917	26.199 27.212	-7.224	1.00	0.00		3A4
ATOM	2453		TYR	354	30.683	27.496	-6.314	1.00	0.00		3A4
ATOM	2454	CZ	TYR	354	31.774	28.004	-7.035	1.00	0.00		3A4
MOTA	2455	OH	TYR	354	31.722	29.310	-7.571	1.00	0.00		3A4
MOTA	2456	C	TYR	354	32.592	22.628	-3.428	1.00	0.00		37.4
ATOM	2457	0	TYR	354	31.575	22.220	-2.892	1.00	0.00		3A4 3A4
ATOM	2458 2459	N CA	LEU	355 355	33.710 33.715	21.867 20.493	-3.466 -2.996	1.00	0.00		3A4
ATOM ATOM	2460	CB	LEU	355	34.970	19.771	-3.512	1.00	0.00		3A4
ATOM	2461	CG	LEU	355	34.521	18.784	-4.631	1.00	0.00		3A4
ATOM	2462		LEU	355	35.547	18.525	-5.749	1.00	0.00		3A4
ATOM	2463	CD2	LEU	355	33.945	17.479	-4.064	1.00	0.00		3A4
ATOM	2464	С	LEU	355	33.573	20.380	-1.485	1.00	0.00		3A4
ATOM	2465	0	LEU	355	32.806	19.570	-0.980	1.00	0.00		3A4 3A4
ATOM ATOM	2466	N CA	ASP ASP	356 356	34.225 34.070	21.283	-0.721 0.714	1.00	0.00		3A4
ATOM	2467 2468	СВ	ASP	356	34.921	22.723	1.144	1.00	0.00		3A4
ATOM	2469	CG	ASP	356	35.819	22.461	2.358	1.00	0.00		3A4
ATOM	2470		ASP	356	35.262	22.182	3.454	1.00	0.00		3A4
ATOM	2471		ASP	356	37.067	22.560	2.214	1.00	0.00		3A4
MOTA	2472	C	ASP	356	32.651	21.700	1.182	1.00	0.00		3A4
ATOM	2473	0	ASP	356 357	32.180 31.928	21.110 22.551	2.149 0.423	1.00	0.00		3A4 3A4
ATOM ATOM	2474 2475	N CA	MET MET	35 <i>1</i> 357	30.540	22.331	0.423	1.00	0.00		3A4
ATOM	2476	СВ	MET	357	30.168	24.100	-0.239	1.00	0.00		3A4
MOTA	2477	CG	MET	357	29.601	25.250	0.627	1.00	0.00		3A4

ATOM	2478	SD	MET	357	30.612	26.763	0.665	1.00	0.00	3A4
ATOM	2479	CE	MET	357	29.381	27.754	1.562	1.00	0.00	3A4
ATOM	2480	С	MET	357	29.62 2	21.737	0.289	1.00	0.00	3A4
ATOM	2481	0	MET	357	28.618	21.519	0.952	1.00	0.00	3A4
ATOM	2482	N	VAL	358	29.995	20.909	-0.714	1.00	0.00	3A4
MOTA	2483	CA	VAL	358	29.302	19.693	-1.096	1.00	0.00	3A4
MOTA	2484	CB	VAL	358	29.848	19.071	-2.374	1.00	0.00	3A4
ATOM	2485		VAL	358	29.224	17.667	-2.681	1.00	0.00	3A4
MOTA	2486		VAL	358	29.530	20.074	-3.459	1.00	0.00	3A4
MOTA	2487	С	VAL	358	29.376	18.671	0.012	1.00	0.00	3A4 3A4
MOTA	2488	0	VAL	358	28.364	18.076	0.363	1.00	0.00	3A4
ATOM	2489	N	VAL	359	30.567 30.783	18.479 17.579	1.758	1.00	0.00	3A4
ATOM	2490 2491	CA CB	VAL VAL	359 359	32.264	17.531	2.146	1.00	0.00	3A4
ATOM ATOM	2492		VAL	359	32.553	16.768	3.459	1.00	0.00	3A4
ATOM	2493		VAL	359	33.043	16.854	1.004	1.00	0.00	3A4
ATOM	2494	c	VAL	359	29.954	17.977	2.962	1.00	0.00	3A4
ATOM	2495	ō	VAL	359	29.303	17.151	3.591	1.00	0.00	3A4
ATOM	2496	N	ASN	360	29.903	19.287	3.263	1.00	0.00	3A4
ATOM	2497	CA	ASN	360	29.117	19.830	4.350	1.00	0.00	3A4
MOTA	2498	CB	ASN	360	29.412	21.328	4.537	1.00	0.00	3A4
MOTA	2499	CG	ASN	360	30.795	21.548	5.189	1.00	0.00	3A4
ATOM	2500	OD1	ASN	360	31.725	20.750	5.080	1.00	0.00	3A4
ATOM	2501		ASN	360	30.946	22.706	5.890	1.00	0.00	3A4
ATOM	2502	С	ASN	360	27.624	19.645	4.147	1.00	0.00	3A4
ATOM	2503	0	ASN	360	26.891	19.274	5.060	1.00	0.00	3A4 3A4
ATOM	2504	И	GLU	361		19.820	2.890 2.527	1.00	0.00	3A4
ATOM	2505	CA	GLU	361 361	25.768 25.458	19.606 20.211	1.139	1.00	0.00	3A4
ATOM ATOM	2506 2507	CB CG	GLU GLU	361	24.026	19.998	0.629	1.00	0.00	3A4
ATOM	2508	CD	GLU	361	22.935	20.638	1.489	1.00	0.00	3A4
ATOM	2509		GLU	361	23.253	21.306	2.504	1.00	0.00	3A4
ATOM	2510		GLU	361	21.740	20.442	1.143	1.00	0.00	3A4
ATOM	2511	С	GLU	361	25.372	18.147	2.553	1.00	0.00	3A4
ATOM	2512	0	GLU	361	24.258	17.809	2.941	1.00	0.00	3A4
ATOM	2513	N	THR	362	26.285	17:210	2.205	1.00	0.00	3A4
ATOM	2514	CA	THR	362	26.034	.15.779		1.00	0.00	3A4
ATOM	2515	CB	THR	362	27.109	14.973	1.573	1.00	0.00	3A4 3A4
ATOM	2516		THR	362	27.154 26.766	15.360 13.462	0.208 1.673	1.00	0.00	3A4
ATOM ATOM	2517 2518	C	THR THR	362 362	25.886	15.303	3.702	1.00	0.00	3A4
ATOM	2519	ŏ	THR	362	24.990	14.527	4.020	1.00	0.00	3A4
ATOM	2520	N	LEU	363	26.722	15.835	4.611	1.00	000	3A4
ATOM	2521	CA	LEU	363	26.677	15.555	6.026	1.00	0.00	3A4
ATOM	2522	СB	LEU	363	27.934	16.102	6.729	1.00	0.00	3A4
ATOM	2523	CG	LEU	363	29.216	15.310	6.428	1.00	0.00	3A4
ATOM	2524		LEU	363	30.434	16.188	6.740	1.00	0.00	3A4
ATOM	2525		LEU	363	29.238	13.981	7.211	1.00	0.00	3A4
ATOM.	2526	C	LEU	363	25.448 24.956	16.157	6.698 7.681	1.00	0.00	3A4 3A4
ATOM	2527 2528	O N	LEU ARG	363 364	24.890	15.614 17.274	6.163	1.00	0.00	3A4
ATOM ATOM	2529	CA	ARG	364	23.659	17.879	6.633	1.00	0.00	3A4
ATOM	2530	СВ	ARG	364	23.446	19.303	6.082	1.00	0.00	3A4
ATOM	2531	CG	ARG	364	22.238			1.00	0.00	3A4
ATOM	2532	CD	ARG	364	22.212	21.544	6.417	1.00	0.00	3A4
ATOM	2533	NE	ARG	364	21.256	22.182	7.393	1.00	0.00	3A4
MOTA	2534	CZ	ARG	364	21.624	22.741	8.595	1.00	0.00	3A4
ATOM	2535		ARG	364	20.663	23.251	9.418	1.00	0.00	3A4
ATOM	2536		ARG	364	22.925	22.809	8.992	1.00	0.00	3A4
ATOM	2537	C	ARG	364	22.463	17.060	6.233	1.00	0.00	3A4 3A4
ATOM	2538	0	ARG	364 365	21.622 22.393	16.711 16.685	7.049 4.940	1.00	0.00	3A4
ATOM ATOM	2539 2540	N CA	LEU LEU	365 365	22.393	15.979	4.384	1.00	0.00	3A4
ATOM	2541	CB	LEU	365	21.247	16.050	2.848	1.00	0.00	3A4
ATOM	2542	CG	LEU	365	19.879	16.592	2.326	1.00	0.00	3A4
ATOM	2543		LEU	365	19.837	16.585	0.811	1.00	0.00	3A4
ATOM	2544		LEU	365	18.607	15.874	2.828	1.00	0.00	3A4
ATOM	2545	C	LEU	365	21.135	14.540	4.810	1.00	0.00	3A4
MOTA	2546	0	LEU	365	20.029	14.082	5.089	1.00	0.00	3A4
ATOM	2547	N	PHE	366	22.252	13.787	4.904	1.00	0.00	3A4
ATOM	2548	CA	PHE	366 366	22.226	12.409	5.376	1.00	0.00	3A4 3A4
ATOM	2549	СВ	PHE	366	22.642	11.385	4.273	1.00	0.00	277

ATOM	2550	CG	PHE	366	21.503	11.244	3.297	1.00	0.00	3A4
ATOM	2551	CD1		366	21.538	11.861	2.035	1.00	0.00	3A4
MOTA	2552	CD2	PHE	366	20.363	10.498	3.651	1.00	0.00	3A4
MOTA	2553	CE1	PHE	366	20.455	11.742	1.150	1.00	0.00	3A4
MOTA	2554	CE2	PHE	366	19.278	10.377	2.773	1.00	0.00	3A4
MOTA	2555	CZ	PHE	366	19.325	11.000	1.520	1.00	0.00	3A4
ATOM	2556	С	PHE	366	23.116	12.273	6.585	1.00	0.00	3A4 3A4
MOTA	2557	0	PHE	366	24.165	11.637	6.497	1.00	0.00	3A4
ATOM	2558	N	PRO	367	22.732	12.795	7.772 9.011	1.00	0.00	3A4
MOTA	2559	CA	PRO	367	23.466 21.498	12.674 13.517	7.993	1.00	0.00	3A4
ATOM	2560	CD CB	PRO PRO	367 367	22.894	13.739	9.935	1.00	0.00	3A4
ATOM ATOM	2561 2562	CG	PRO	367	21.461	13.878	9.463	1.00	0.00	3A4
ATOM	2563	C	PRO	367	23,332	11.269	9.536	1.00	0.00	3A4
ATOM	2564	ŏ	PRO	367	22.246	10.779	9.824	1.00	0.00	3A4
ATOM	2565	N	ILE	368	24.476	10.572	9.569	1.00	0.00	3A4
ATOM	2566	CA	ILE	368	24.602	9.143	9.718	1.00	0.00	3A4
ATOM	2567	CB	ILE	368	25.992	8.818	9.131	1.00	0.00	3A4
ATOM	2568	CG2	ILE	368	27.160	9.306	10.024	1.00	0.00	3A4 .
MOTA	2569		ILE	368	26.230	7.413	8.553	1.00	0.00	3A4 3A4
ATOM	2570	CD	ILE	368	26.421	6.268	9.546	1.00	0.00	3A4
ATOM	2571	C	ILE	368	24.406	8.654	11.153	1.00	0.00	3A4
ATOM	2572	0	ILE	368	24.024	7.515 9.530	11.392 12.146	1.00	0.00	3A4
MOTA	2573	N	ALA	369	24.661 24.719	9.183	13.542	1.00	0.00	3A4
ATOM	2574	CA CB	ALA ALA	369 369	26.067	9.640	14.141	1.00	0.00	3A4
ATOM ATOM	2575 2576	С	ALA	369	23.654	9.859	14.360	1.00	0.00	3A4
ATOM	2577	ŏ	ALA	369	23.267	10.991	14.104	1.00	0.00	3A4 `
ATOM	2578	N	MET	370	23.265	9.221	15.511	1.00	0.00	3A4
ATOM	2579	CA	MET	370	22.422	9.803	16.560	1.00	0.00	3A4
ATOM	2580	CB	MET	370	20.964	9.264	16.470	1.00	0.00	3A4
MOTA	2581	CG	MET	370	19.910	10.113	17.209	1.00	0.00	· 3A4
MOTA	2582	SD	MET	370	18.173	9.663	16.885	1.00	0.00	3A4
MOTA	2583	CE	MET	370	18.081	10.195	15.146	1.00	0.00	3A4
ATOM	2584	С	MET	370	23.062	9.512	17.921	1.00	0.00	3A4 3A4
ATOM	2585	0	MET	370	23.884	8.603 10.299	18.029 18.992	1.00 1.00	0.00	3A4
ATOM	2586	N	ARG	371	22.711 23.356	10.233	20.307	1.00	0.00	3A4
ATOM	2587 2588	CA CB	ARG ARG	371 371	24.430	11.405	20.437	1.00	0.00	3A4
ATOM ATOM	2589	CG	ARG	371	23.944	12.828	20.099	1.00	0.00	3A4
ATOM	2590	CD	ARG	371	25.049	13.888	20.216	1.00	0.00	· 3A4
ATOM	2591	NE	ARG	371	24.503	15.208	19.738	1.00	0.00	3A4
ATOM	2592	CZ	ARG	371	25.012	16.428	20.108	1.00	0.00	3A4
ATOM	2593	NH1	ARG	371	24.468	17.561	19.575	1.00	0.00	3A4
MOTA	2594	NH2	ARG	371	26.049	16.546	20.988	1.00	0.00	3A4
MOTA	2595	С	ARG	371	22.333	10.392	21.438	1.00	0.00	3A4
MOTA	2596	0	ARG	. 371	21.181	10.760	21.216	1.00	0.00	3A4 3A4
	2597	N	LEU	372	22.776	10.045	22.692	1.00	0.00	3A4 3A4
ATOM	2598	CA	LEU	372.	22.016 21.964	9.951 8.482	23.936 24.512	1.00	0.00	3A4
ATOM	2599 2600	CB CG	LEU	372 372	21.345	7.343	23.661	1.00	0.00	3A4
ATOM ATOM	2601		LEU	372	19.908	7.641	23.227	1.00	0.00	3A4
ATOM	2602		LEU	372	22.216	6.816	22.501	1.00	0.00	3A4
ATOM	2603	c	LEU	372	22.693	10.771	25.005	1.00	0.00	3A4
ATOM	2604	ō	LEU	372	23.899	11.003	24.975	1.00	0.00	3A4
ATOM	2605	N	GLU	373	21.900	11.155	26.021	1.00	0.00	3A4
MOTA	2606	CA	GLU	373	22.322	11.807	27.237	1.00	0.00	3A4
ATOM	2607	СB	GLU	373	22.131	13.344	27.172	1.00	0.00	3A4
ATOM	2608	CG	GLU	373	23.197	14.057	26.329	1.00	0.00	3A4 3A4
ATOM	2609	CD	GLU	373	23.009	15.577	26.343	1.00	0.00	3A4
MOTA	2610		GLU	373	23.722	16.250	25.553 27.128	1.00	0.00	3A4
ATOM	2611	OE2		373 373	22.167 21.466	16.090 11.241	28.351	1.00	0.00	3A4
MOTA	2612	0	GLU	373 373	20.387	10.695	28.121	1.00	0.00	3A4
ATOM ATOM	2613 2614	N	ARG	374	21.930	11.386	29.612	1.00	0.00	3A4
ATOM	2615	CA	ARG	374	21.138	11.043	30.774	1.00	0.00	3A4
ATOM	2616	СВ	ARG	374	21.532	9.678	31.420	1.00	0.00	3A4
ATOM	2617	CG	ARG	374	22.371	9.595	32.715	1.00	0.00	3A4
ATOM	2618	CD	ARG	374	21.558	9.546	34.018	1.00	0.00	3A4
ATOM	2619	NE	ARG	374	22.476	9.916	35.152	1.00	0.00	3A4
ATOM	2620	CZ	ARG	374	22.249	9.595	36.465	1.00	0.00	3A4
MOTA	2621	NHl	ARG	374	23.147	10.010	37.405	1.00	0.00	3A4

ATOM	2622	NH2	ARG	374	21.156	8.879	36.860	1.00	0.00	3A4
ATOM	2623	С	ARG	374	21.272	12.200	31.721	1.00	0.00	3A4
ATOM	2624	0	ARG	374	22.360	12.720	31.947	1.00	0.00	3A4
ATOM	2625	N	VAL	375	20.152	12.629	32.340	1.00	0.00	3A4 3A4
ATOM	2626	CA	VAL	375 375	20.085 18.651	13.742 14.239	33.272 33.344	1.00	0.00	3A4
ATOM ATOM	2627 2628	CB	VAL VAL	375	18.283	15.175	34.420	1.00	0.00	3A4
ATOM	2629		VAL	375	18.394	14.888	31.964	1.00	0.00	3A4
ATOM	2630	c	VAL	375	20.606	13.314	34.625	1.00	0.00	3A4
ATOM	2631	0	VAL	375	20.173	12.325	35.197	1.00	0.00	3A4
MOTA	2632	N	CYS	376	21.593	14.058	35.166	1.00	0.00	3A4
MOTA	2633	CA	CYS	376	22.269	13.722	36.404	1.00	0.00	3A4 3A4
ATOM	2634	CB	CYS	376 376	23.708 24.721	14.284	36.408 35.165	1.00	0.00	3A4
ATOM ATOM	2635 2636	SG C	CYS	376	21.525	14.230	37.618	1.00	0.00	
MOTA	2637	ŏ	CYS	376	21.699	13.713	38.720	1.00	0.00	3A4
ATOM	2638	N	LYS	377	20.691	15.268	37.426	1.00	0.00	3A4
MOTA	2639	CA	LYS	377	19.982	15.944	38.480	1.00	0.00	3A4
ATOM	2640	CB	LYS	377	20.773	17.167	38.996	1.00	0.00	3A4
ATOM	2641	CG	LYS	377	22.008	16.876	39.867 41.198	1.00	0.00 0.00	3A4 3A4
ATOM ATOM	2642 2643	CD	LYS LYS	377 3 7 7	21.695 22.947	16.179 15.957	42.056	1.00	0.00	3A4
ATOM	2644	NZ	LYS	377	22.604	15.293	43.336	1.00	0.00	3A4
ATOM	2645	c	LYS	377	18.735	16.448	37.827	1.00	0.00	3A4
ATOM	2646	0	LYS	377	18.689	16.603	36.617	1.00	0.00	3A4
ATOM	2647	N	LYS	378	17.690	16.839	38.593	1.00	0.00	3A4
ATOM	2648	CA	LYS	378	16.465	17.414	38.063 39.177	1.00	0.00	3A4 3A4
ATOM ATOM	2649 2650	CB CG	LYS LYS	378 378	15.419 15.088	17.607 16.287	39.895	1.00	0.00	3A4
ATOM	2651	CD	LYS	378	14.017	16.418	40.984	1.00	0.00	3A4
ATOM	2652	CE	LYS	378	13.613	15.082	41.625	1.00	0.00	3A4
MOTA	2653	NZ	LYS	378	14.747	14.462	42.352	1.00	0.00	3A4
MOTA	2654	C	LYS	378	16.741	18.741	37.382	1.00	0.00	3A4
ATOM	2655	0	LYS	378	17.545 16.172	19.524 18.960	37.877 36.183	1.00	0.00	3A4 3A4
ATOM ATOM	2656 2657	N CA	ASP ASP	379 379	16.172	20.125	35.394	1.00	0.00	3A4
ATOM	2658	CB	ASP	379	17.706	19.925	34.443	1.00	0.00	3A4
ATOM	2659	CG	ASP	379	17.527	19.059	33.183	1.00	0.00	3A4
ATOM	2660		ASP	379	17.455	17.817	33.330	1.00	0.00	3A4
ATON	2661		ASP	379	17.475	19.634	32.063	1.00	0.00	3A4 3A4
ATOM	2662	C	ASP ASP	379 379	15.250 14.333	20.543 19.776	34.652 34.415	1.00	0.00	3A4
ATOM ATOM	2663 2664	O N	VAL	380	15.216	21.819	34.247	1.00	0.00	3A4
ATOM	2665	CA	VAL	380	14.098	22.398	33.548	1.00	0.00	3A4
ATOM	2666	СВ	VAL	380	13.450	23.491	34.376	1.00	0.00	3A4
ATOM	2667		VAL	380	12.212	24.040	33.665	1.00	0.00	3A4
ATOM	2668		VAL	380	13.057	22.943	35.763	1.00	0.00	3A4 3A4
MOTA MOTA	2669 2670	C O	VAL	380 380	14.659 15.521	22.869 23.743	32.227 32.201	1.00	0.00	3A4.
ATOM	2671	N	GLU	381	14.219	22.259	31.107	1.00	0.00	3A4
ATOM	2672	CA	GLU	381	14.653	22.560	29.760	1.00	0.00	3A4
MOTA	2673	СВ	GLU	381	15.044	21.298	28.989	1.00	0.00	3A4
ATOM	2674	CG	GLU	381	15.995	21.611	27.810	1.00	0.00	3A4
ATOM	2675	CD	GLU	381	16.331 17.063	20.375	26.965 25.958	1.00	0.00	3A4 3A4
ATOM ATOM	2676 2677		GLU	381 381	15.873	19.246	27.284	1.00	0.00	3A4
ATOM	2678	c	GLU	381	13.495	23.231	29.052	1.00	0.00	3A4
MOTA	2679	0.	GLU	381	12.355	22.802	29.042	1.00	0.00	3A4
ATOM	2680	N	ILE	382	13.715	24.405	28.468	1.00	0.00	3A4
ATOM	2681	CA	ILE	382	12.690	25.313	27.960 26.638	1.00	0.00	3A4 3A4
MOTA	2682 2683	CB	ILE	382 382	11.956 10.525	24.945 25.549	26.472	1.00	0.00	3A4
ATOM ATOM	2684		ILE	382	12.874	25.434	25.467	1.00	0.00	3A4
ATOM	2685	CD	ILE	382	12.229	25.497	24.082	1.00	0.00	3A4
MOTA	2686	С	ILE	382	11.919	25.809	29.163	1.00	0.00	3A4
MOTA	2687	0	ILE	382	12.497	26.469	29.990	1.00	0.00	3A4
ATOM	2688	N	ASN	383	10.722	25.435	29.490	1.00	0.00	3A4 3A4
MOTA MOTA	2689 2690	CA CB	ASN ASN	383 383	10.349 9.806	25.838 27.330	30.866 30.959	1.00	0.00	3A4
ATOM	2691	CG	ASN	383	9.693	27.860	32.407	1.00	0.00	3A4
ATOM	2692		ASN	383	8.596	28.169	32.869	1.00	0.00	3A4
ATOM	2693		ASN	383	10.843	27.967	33.129	1.00	0.00	3A4

ATOM	2694	С	ASN	383	9.349	24.945	31.284	1.00	0.00	3A4
ATOM	2695	0	ASN	383	8.160	25.107	30.993	1.00	0.00	3A4
MOTA	2696	N	GLY	384	9.485	23.892	32.102	1.00	0.00	3A4
ATOM	2697	CA	GLY	384	8.315 8.276	22.984 22.292	32.156 30.798	1.00	0.00	3A4 3A4
ATOM ATOM	2698 2699	С 0	GLY	384 384	7.285	21.764	30.798	1.00	0.00	3A4
ATOM	2700	N	MET	385	9.600	22.252	30.331	1.00	0.00	3A4
ATOM	2701	ÇA	MET	385	9.904	20.858	30.491	1.00	0.00	3A4
ATOM	2702	СВ	MET	385	10.648	20.273	29.245	1.00	0.00	3A4
ATOM	2703	CG	MET	385	10.078	18.932	28.749	1.00	0.00	3A4 3A4
ATOM	2704 2705	SD CE	MET MET	385 385	10.271 8.674	17.522 16.747	29.885 29.504	1.00	0.00	3A4 3A4
ATOM ATOM	2706	C	MET	385	10.673	20.574	31.772	1.00	0.00	3A4
ATOM	2707	ō	MET	385	11.823	20.957	31.867	1.00	0.00	3A4
ATOM	2708	N	PHE	386	10.077	19.903	32.767	1.00	0.00	3A4
ATOM	2709	CA	PHE	386	10.786	19.416	33.933	1.00	0.00	3A4 3A4
ATOM	2710 2711	CB CG	PHE	386 386	9.854 10.561	19.471 19.327	35.160 36.492	1.00	0.00	3A4
ATOM ATOM	2711		PHE	386	10.905	20.467	37.242	1.00	0.00	3A4
ATOM	2713		PHE	386	10.861	18.057	37.026	1.00	0.00	3A4
MOTA	2714	CE1	PHE	386	11.556	20.349	38.477	1.00	0.00	3A4
ATOM	2715		PHE	386	11.512	17.931	38.260	1.00	0.00	3A4
MOTA	2716	cz	PHE	386	11.859 11.245	19.080 17.997	38.985 33.650	1.00	0.00	3A4 3A4
ATOM ATOM	2717 2718	С 0	PHE PHE	386 386	10.434	17.097	33.442	1.00	0.00	3A4
ATOM	2719	N	ILE	387	12.579	17.797	33.622	1.00	0.00	3A4
ATOM	2720	CA	ILE	387	13.234	16.542	33.348	1.00	0.00	3A4
ATOM	2721	CB	ILE	387	14.381	16.682	32.335	1.00	0.00	3A4
MOTA	2722		ILE	387	14.760	15.256	31.874	1.00	0.00	3A4 3A4
MOTA MOTA	2723 2724	CD	ILE	387 387	13.940 14.996	17.566 17.732	31.142 30.052	1.00	0.00	3A4
ATOM	2725	c	ILE	387	13.712	16.037	34.699	1.00	0.00	3A4
MOTA	2726	0	ILE	387	14.542	16.701	35.311	1.00	0.00	3A4
MOTA	2727	N	PRO	388	13.230	14.898	35.231	1.00	0.00	3A4
MOTA	2728	CA	PRO	388	13.741	14.297	36.449	1.00	0.00	3A4 3A4
ATOM ATOM	2729 2730	CD CB	PRO PRO	388 388	11.827 12.685	14.522 13.264	35.038 36.864	1.00	0.00	3A4
ATOM	2731	CG	PRO	388	11.381	13.833	36.327	1.00	0.00	3A4
ATOM	2732	C	PRO	388 -	15.090	13.656	36.297	1.00	0.00	3A4
MOTA	2733	0	PRO	388	15.481	13.246	35.212	1.00	0.00	3A4
ATOM	2734	И	LYS	389	15.825	13.516	37.416	1.00	0.00	3A4 3A4
ATOM ATOM	2735 2736	CA CB	LYS LYS	389 389	17.102 17.661	12.839 12.891	37.479 38.918	1.00	0.00	3A4
ATOM	2737	ÇG	LYS	389	16.754	12.453	40.092	1.00	0.00	3A4
ATOM	2738	CD	LYS	389	16.878	10.984	40.532	1.00	0.00	3A4
MOTA	2739	CE	LYS	389	16.079	10.653	41.802	1.00	0.00	3A4
ATOM	2740 2741	NZ C	LYS	389 389	14.624 16.984	10.849 11.412	41.589 37.009	1.00	0.00	3A4 3A4
ATOM ATOM	2741	ò	LYS	389	15.997	10.745	37.301	1.00	0.00	3A4
ATOM	2743	N	GLY	390	17.932	10.973	36.172	1.00	0.00	3A4
ATOM	2744	ÇA	GLY	390	17.963	9.654	35.593	1.00	0.00	3A4
MOTA	2745	C	GLY	390	17.174	9.470	34.332	1.00	0.00	3A4 3A4
ATOM ATOM	2746 2747	0	GLY TRP	390 391	17.046 16.619	8.351 10.571	33.839 33.769	1.00	0.00	3A4
ATOM	2748	N CA	TRP	391	15.850	10.544	32.546	1.00	0.00	3A4
ATOM	2749	СВ	TRP	391	14.930	11.760	32.448	1.00	0.00	3A4
MOTA	2750	ÇG	TRP	391	13.571	11.608	33.100	1.00	0.00	3A4
ATOM	2751		TRP	391	13.050	10.792	34.187	1.00	0.00	3A4
ATOM ATOM	2752 2753		TRP TRP	391 391	12.458 11.305	12.068 11.618	32.439 33.025	1.00	0.00	3A4 3A4
ATOM	2754		TRP	391	11.634	10.839	34.102	1.00	0.00	3A4
ATOM	2755	CE3	TRP	391	13.655	10.032	35.188	1.00	0.00	'3A4
ATOM	2756		TRP	391	10.825	10.153	35.005	1.00	0.00	3A4
ATOM	2757		TRP	391	12.843	9.345	36.102	1.00	0.00	3A4 3A4
ATOM ATOM	2758 2759	CH2	TRP	391 391	11.446 16.783	9.404 10.563	36.011 31.369	1.00	0.00	3A4 3A4
ATOM	2760 ·	Ö	TRP	391	17.769	11.289	31.371	1.00	0.00	3A4
ATOM	2761	N	VAL	392	16.466	9.736	30.350	1.00	0.00	3A4
MOTA	2762	CA	VAL	392	17.263	9.564	29.159	1.00	0.00	3A4
ATOM	2763	CB	VAL	392	17.270	8.105	28.700	1.00	0.00	3A4 3A4
MOTA MOTA	2764 2765		VAL VAL	392 392	17.957 17.984	7.898 7.270	27.322 29.787	1.00	0.00	3A4
.11 013	2.05		4 4 4 4 4 4 4	32	20.007					

ATOM	2766	С	VAL	392	16.723	10.497	28.110	1.00	0.00	3A4
MOTA	2767	0	VAL	392	15.519	10.598	27.908	1.00	0.00	3A4
ATOM	2768	N	VAL	393	17.636	11.234	27.453	1.00	0.00	3A4
MOTA	2769	CA	VAL VAL	393 .	17.333	12.226	26.455 26.868	1.00	0.00	3A4 3A4
ATOM ATOM	2770 2771	CB	VAL	393 393	17.828 17.556	13.610 14.652	25.780	1.00	0.00	3A4
ATOM	2772		VAL	393	17.145	14.023	28.194	1.00	0.00	3A4
MOTA	2773	С	VAL	393	17.993	11.735	25.192	1.00	0.00	3A4
MOTA	2774	0	VAL	393	19.147	11.327	25.196	1.00	0.00	3A4
MOTA	2775	N	MET	394	17.251	11.776	24.072	1.00	0.00	3A4
MOTA	2776	CA	MET	394	17.726	11.439	22.757 22.065	1.00	0.00	3A4 3A4
ATOM ATOM	2777 _. 2778	CB CG	MET	394 394	16.799 16.558	10.393 9.106	22.860	1.00	0.00	3A4
ATOM	2779	SD	MET	394	15.673	7.800	21.946	1.00	0.00	3A4
MOTA	2780	CE	MET	394	16.910	7.426	20.666	1.00	0.00	3A4
MOTA	2781	С	MET	394	17.772	12.724	21.991	1.00	0.00	3A4
MOTA	2782	0	MET	394	16.799	13.464	21.947	1.00	0.00	3A4
ATOM ATOM	2783 2784	N CA	ILE	395 395	18.916 19.139	13.023 14.208	21.347 20.554	1.00	0.00	3A4 3A4
ATOM	2785	CB	ILE	395	20.476	14.837	20.956	1.00	0.00	3A4
ATOM	2786		ILE	395	21.095	15.840	19.965	1.00	0.00	3A4
ATOM	2787	CG1	ILE	395	20.413	15.442	22.374	1.00	0.00	3A4
MOTA	2788	CD	ILE	395	20.802	14.496	23.518	1.00	0.00	3A4
ATOM	2789	C	ILE	395	19.146	13.747	19.102	1.00	0.00	3A4
MOTA MOTA	2790 2791	о И	ILE PRO	395 396	20.160 18.048	13.239 13.907	18.627 18.342	1.00	0.00	3A4 3A4
ATOM	2792	CA	PRO	396	18.027	13.792	16.906	1.00	0.00	3A4
ATOM	2793	CD	PRO	396	16.755	13.448	18.870	1.00	0.00	3A4
MOTA	2794	СВ	PRO	396	16.531	13.829	16.546	1.00	0.00	3A4
MOTA	2795	CG	PRO	396	15.857	13.097	17.687	1.00	0.00	3A4
MOTA MOTA	2796 2797	С О	PRO PRO	396 396	18.776 18.239	14.889 15.950	16.173 15.861	1.00	0.00	3A4 3A4
ATOM	2798	N	SER	397	20.048	14.601	15.825	1.00	0.00	3A4
ATOM	2799	CA	SER	397	20.904	15.470	15.055	1.00	0.00	3A4
MOTA	2800	CB	SER	397	22.360	14.989	15.079	1.00	0.00	3A4
ATOM	2801	OG	SER	397	22.500	13.601	14.800	1.00	0.00	3A4
MOTA	2802	С 0	SER	397 397	20.417 20.522	15.595 16.640	13.635 13.023	1.00	0.00	3A4 3A4
ATOM ATOM	2803 2804	N	SER TYR	398	19.766	14.539	13.106	1.00	0.00	3A4
ATOM	2805	CA	TYR	398	19.026	14.496	11.862	1.00	0.00	3A4
ATOM	2806	CB .	TYR	398	18.323	13.079	11.799	1.00	0.00	3A4
ATOM	2807	CG	TYR	398	18.447	12.353	10.483	1.00	0.00	3A4
ATOM	2808	CD1		398	19.004	11.056	10.456	1.00	0.00	3A4
ATOM ATOM	2809 2810	CD2 CE1		398 398	18.041 19.153	12.935 10.357	9.266 9.251	1.00 1.00	0.00	3A4 3A4
ATOM	2811	CE2		398	18.216	12.249	8.058	1.00	0.00	3A4
MOTA	2812	CZ	TYR	398	. 18.763	10.958	8.048	1.00	0.00	3A4
ATOM	2813	ОН	TYR	398	18.924	10.266	6.829	1.00	0.00	3A4
ATOM	2814	C	TYR	398	17.923	15.540	11.741	1.00	0.00	3A4
ATOM ATOM	2815 2816	O N	TYR ALA	398 399	17.730 17.184	16.207 15.730	10.728 12.853	1.00	0.00	3A4 3A4
ATOM	2817	CA	ALA	399	16.116	16.686	12.969	1.00	0.00	3A4
ATOM	2818	CB	ALA	399	15.263	16.409	14.206	1.00	0.00	3A4
ATOM	2819	С	ALA	399	16.594	18.122	13.028	1.00	0.00	3A4
ATOM	2820	0	ALA	399	15.939	19.008	12.501	1.00	0.00	3A4
ATOM ATOM	2821 2822	N CA	LEU	400 400	17.795 18.426	18.377 19.687	13.599 13.645	1.00 1.00	0.00	3A4 3A4
ATOM	2823	СВ	LEU	400	19.762	19.647	14.448	1.00	0.00	3A4
ATOM	2824	CG	LEU	400	19.694	19.664	15.956	1.00	0.00	3A4
MOTA	2825	CD1		400	20.663	20.773	16.433	1.00	0.00	3A4
ATOM	2826	CD2		400	18.244	19.759	16.433	1.00	0.00	3A4
MOTA MOTA	2827 2828	С 0	LEU LEU	400 400	18.832 18.639	20.202 21.368	12.285 11.954	1.00 1.00	0.00	3A4 3A4
ATOM	2829	N	HIS	401	19.402	19.298	11.465	1.00	0.00	3A4
ATOM	2830	CA	HIS	401	19.852	19.556	10.124	1.00	0.00	3A4
MOTA	2831	ND1	HIS	401	22.332	16.943	10.714	1.00	0.00	3A4
ATOM	2832	CG	HIS	401	21.917	18.117	10.143	1.00	0.00	3A4
ATOM ATOM	2833 2834	CB NE2	HIS	401 401	20.572 24.123	18.319 18.219	9.559 10.505	1.00	0.00	3A4 3A4
ATOM	2835	CD2		401	23.023	18.219	10.505	1.00	0.00	3A4 3A4
ATOM	2836	CE1		401	23.659	17.057	10.914	1.00	0.00	3A4
MOTA	2837	С	HIS	401	18.745	19.836	9.125	1.00	0.00	3A4

MOTA	2838	0	HIS	401	18.970	20.398	8.056	1.00	0.00		3A4
MOTA	2839	N	ARG	402	17.513	19.410	9.474	1.00	0.00		3A4 3A4
ATOM	2840	CA	ARG	402 402	16.350 15.632	19.558 18.220	8.644 8.410	1.00	0.00		3A4
ATOM ATOM	2841 2842	CB CG	ARG	402	16.476	17.220	7.607	1.00	0.00		3A4
ATOM	2843	CD	ARG	402	15.663	15.992	7.176	1.00	0.00		3A4
ATOM	2844	NE	ARG	402	16.519	15.105	6.308	1.00	0.00		3A4
MOTA	2845	CZ	ARG	402	16.028	14.373	5.254	1.00	0.00		3A4 3A4
ATOM	2846	NH1		402	16.860	13.518 14.465	4.593 4.853	1.00	0.00		3A4
ATOM	2847 2848	NH2 C	ARG	402 402	14.725 15.378	20.553	9.211	1.00	0.00		3A4
ATOM ATOM	2849	Ö	ARG	402	14.224	20.625	8.790	1.00	0.00		3A4
ATOM	2850	N	ASP	403	15.839	21.391	10.171	1.00	0.00		3A4
MOTA	2851	CA	ASP	403	15.031	22.422	10.772	1.00	0.00		3A4 3A4
ATOM	2852	СВ	ASP	403	15.642 14.530	22.973 23.734	12.085 12.847	1.00	0.00		3A4
ATOM	2853	CG	ASP ASP	403 403	14.530	24.806	12.394	1.00	0.00		3A4
ATOM ATOM	2854 2855		ASP	403	13.981	23.160	13.823	1.00	0.00		3A4
ATOM	2856	C	ASP	403	14.822	23.549	9.771	1.00	0.00		3A4
ATOM	2857	0	ASP	403	15.805	24.148	9.348	1.00	0.00		3A4
ATOM	2858	N	PRO	404	13.575	23.872	9.387 8.377	1.00	0.00		3A4 3A4
ATOM	2859	CA	PRO PRO	404 404	13.256 12.350	24.866 23.288	9.945	1.00	0.00		3A4
ATOM ATOM	2860 2861	CD CB	PRO	404	11.749	24.727	8.133	1.00	0.00		3A4
ATOM	2862	CG	PRO	404	11.195	24.161	9.445	1.00	0.00		3A4
ATOM	2863	С	PRO	404	13.582	26.287	8.784	1.00	0.00		3A4
ATOM	2864	0	PRO	404	13.786	27.122	7.915 10.092	1.00	0.00		3A4 3A4
ATOM	2865	N	LYS LYS	405 405	13.702 14.102	26.594 27.890	10.032	1.00	0.00		3A4
ATOM ATOM	2866 2867	CA CB	LYS	405	13.708	28.082	12.078	1.00	0.00		3A4
ATOM	2868	CG	LYS	405	12.230	27.779	12.361	1.00	0.00		3A4
ATOM	2869	CD	LYS	405	11.862	27.931	13.843	1.00	0.00		3A4 3A4
ATOM	2870	CE	LYS	405	10.437	27.465	14.181 13.467	1.00	0.00		3A4
ATOM	2871	NZ C	LYS	405 405	9.420 15.589	28.274 28.111	10.451	1.00	0.00		3A4
ATOM ATOM	2872 2873	ò	LYS	105	16.040	29.247	10.435	1.00	0.00		3A4
ATOM	2874	N	TYR	406	16.387	27.031	10.326	1.00	0.00		3A4
MOTA	2875	CA	TYR	406	17.828	27.082	10.196	1.00	0.00		3A4 3A4
ATOM	2876	CB	TYR	406	18.501 18.818	25.978 26.481	11.073 12.466	1.00	0.00		3A4
ATOM ATOM	287 7 2878	CG	TYR TYR	406 406	17.845	27.049	13.316	1.00	0.00		3A4
ATOM	2879		TYR	406	20.123	26.324	12.973	1.00	0.00		3A4
MOTA	2880		TYR	406	18.180	27.502	14.601	1.00	0.00		3A4
MOTA	2881	CE2		406	20.465	26.758	14.261	1.00	0.00	•	3A4 3A4
ATOM	2882	CZ	TYR TYR	406 406	19.493 19.831	27.354 27.781	15.076 16.379	1.00	0.00		3A4
ATOM ATOM	2883 2884	OH C	TYR	406	18.238	26.911	8.742	1.00	0.00		3A4
ATOM	2885	ŏ	TYR	406	19.185	27.556	8.293	1.00	0.00		3A4
MOTA	2886	N	TRP	407.	17.542	26.030	7.986	1.00	0.00		3A4
ATOM	2887	CA	TRP	407	17.869	25.728	6.609 6.460	1.00	0.00		3A4 3A4
ATOM	2888 2889	CB CG	TRP TRP	407 407	18.602 19.890	24.364 24.534	5.666	1.00	0.00		3A4
ATOM ATOM	2890		TRP	407	20.082	24.159	4.293	1.00	0.00		3A4
MOTA	2891		TRP	407	21.050	25.141	6.063	1.00	0.00		3A4
MOTA	2892		TRP	407	21.981	25.110	5.052	1.00	0.00		3A4 3A4
MOTA	2893		TRP	407	21.405 19.231	24.521 23.566	3.948 3.365	1.00	0.00		3A4
MOTA MOTA	2894 2895		TRP TRP	407 407	21.902	24.280	2.673	1.00	0.00		3A4
ATOM	2896		TRP	407	19.728	23.326	2.076	1.00	0.00		3A4
ATOM	2897		TRP	407	21.046	23.678	1.741	1.00	0.00		3A4
ATOM	2898	С	TRP	407	16.592	25.684	5.809	1.00	0.00		3A4 3A4
ATOM	2899	0	TRP	407 408	15.735 16.454	24.831 26.581	6.029 4.791	1.00	0.00		3A4
MOTA MOTA	2900 2901	N CA	THR THR	408	15.311	26.691	3.895	1.00	0.00		3A4
MOTA	2902	СВ	THR	408	15.211	28.071	3.263	1.00	0.00		3A4
ATOM	2903	OG1	THR	408	16.432	28.505	2.662	1.00	0.00		3A4
MOTA	2904		THR		14.818	29.070	4.376 2.839	1.00	0.00		3A4 3A4
MOTA	2905 2906	Ç	THR THR		15.392 16.472	25.598 25.245	2.839	1.00	0.00		3A4
MOTA MOTA	2906	O N	GLU	408	14.235	24.987	2.499	1.00			3A4
ATOM	2908	CA	GLU		14.103	23.803	1.664	1.00	0.00		3A4
MOTA	2909	СВ	GLU		14.330	24.118	0.167	1.00	0.00		3A4

ATOM	2910	CG	GLU	409	13.370	25.190	-0.379	1.00	0.00	3A4
MOTA	2911	CD	GLU	409	13.625	25.385	-1.878	1.00	0.00	3A4
ATOM	2912			409	12.698	25.099	-2.683	1.00	0.00	3A4 3A4
ATOM	2913		GLU	409 409	14.752 15.001	25.821 22.657	-2.236 2.097	1.00	0.00	3A4
ATOM ATOM	2914 2915	С 0	GLU	409	15.858	22.218	1.334	1.00	0.00	3A4
MOTA	2916	N	PRO	410	14.886	22.233	3.369	1.00	0.00	3A4
ATOM	2917	CA	PRO	410	15.857	21.388	4.073	1.00	0.00	3A4
ATOM	2918	CD	PRO	410	13.663	22.414	4.165	1.00	0.00	3A4 3A4
ATOM	2919	CB	PRO	410	15.298 13.783	21.307 21.467	5.504 5.357	1.00	0.00 0.00	3A4
ATOM ATOM	2920 2921	CG C	PRO PRO	410 410	16.013	20.007	3.463	1.00	0.00	3A4
ATOM	2922	ŏ	PRO	410	17.048	19.368	3.620	1.00	0.00	3A4
ATOM.	2923	N	GLU	411	15.001	19.530	2.723	1.00	0.00	3A4
ATOM	2924	CA	GLU	411	15.007	18.249	2.086 2.041	1.00	0.00	3A4 3A4
ATOM	2925	CB	GLU	411	13.575 12.398	17.671 18.662	1.868	1.00	0.00	3A4
ATOM ATOM	2926 2927	CG CD	GLU	411 411	12.395	19.342	0.498	1.00	0.00	3A4
ATOM	2928		GLU	411	12.459	20.600	0.464	1.00	0.00	3A4
ATOM	2929		GLU	411	12.316	18.616	-0.530	1.00	0.00	3A4
MOTA	2930	С	GLU	411	15.637	18.272	0.712	1.00	0.00	3A4 3A4
MOTA	2931	0	GLU	411 412	15.745 16.093	17.227 19.439	0.076 0.214	1.00	0.00	3A4
ATOM ATOM	2932 2933	N CA	LYS LYS	412	16.747	19.560	-1.069	1.00	0.00	3A4
ATOM	2934	СВ	LYS	412	16.319	20.855	-1.798	1.00	0.00	3A4
ATOM	2935	CG	LYS	412	14.842	20.918	-2.228	1.00	0.00	3A4
ATOM	2936	CD	LYS	412	14.489	20.264	-3.577	1.00	0.00	3A4 3A4
ATOM	2937	CE	LYS	412	14.483 13.990	18.726 18.220	-3.601 -4.904	1.00	0.00	3A4
ATOM ATOM	2938 2939	NZ C	LYS LYS	412 412	18.246	19.556	-0.876	1.00	0.00	3A4
MOTA	2940	Ö	LYS	412	18.788	20.180	0.031	1.00	0.00	3A4
ATOM	2941	N	PHE	413	18.970	18.849	-1.771	1.00	0.00	3A4
ATOM	2942	CA	PHE	413	20.413	18.790	-1.784	1.00	0.00	3A4 3A4
ATOM	2943	CB	PHE	. 413 413	20.897 22.398	17.450 17.294	-2.401 -2.423	1.00	0.00	3A4
ATOM ATOM	2944 · 2945	CG CD1	PHE	413	23.168	17.227	-1.254	1.00	0.00	3A4
ATOM	2946		PHE	413	23.046	17.095	-3.661	1.00	0.00	3A4
ATOM	2947		PHE	413	24.550	16.999	-1.315	1.00	0.00	3A4
ATOM	2948		PHE	413	24.421	16.834 16.794	-3.726 -2.550	1.00	0.00 0.00	3A4 3A4
ATOM	2949 2950	CZ C	PHE	413 413	25.177 20.891	19.968	-2.586	1.00	0.00	3A4
ATOM ATOM	2951	ŏ	PHE	413	20.724	20.009	-3.801	1.00	0.00	3A4
ATOM	2952	N	LEU	414	21.483	20.957	-1.901	1.00	0.00	3A4
ATOM	2953	CA	LEU	414	21.933	22.177	-2.522	1.00	0.00	3A4. 3A4
ATOM	2954	CB	LEU	414 414	20.902 21.169	23.301 24.700	-2.306 -2.902	1.00	0.00	3A4
ATOM ATOM	2955 2956	CG CD1	LEU	414	21.261	24.685	-4.441	1.00	0.00	3A4
ATOM	2957		LEU	414	20.079	25.663	-2.388	1.00	0.00	3A4
ATOM	2958	С	LEU	414	23.275	22.553	-1.966	1.00	0.00	3A4. 3A4
ATOM	2959	0	LEU	414 .	23.343 24.394	23.031 22.396	-0.834 -2.681	1.00	0.00	3A4
ATOM ATOM	2960 2961	N CA	PRO PRO	415 415	25.721	22.710	-2.165	1.00	0.00	3A4
ATOM	2962	CD	PRO	415	24.457	21.932	-4.069	1.00	0.00	3A4
ATOM	2963	СВ	PRO	415	26.676	22.158	-3.227	1.00	0.00	3A4
ATOM	2964	CG	PRO	415	25.882	22.244	-4.535	1.00	0.00	3A4 3A4
ATOM	2965 2966	С 0	PRO PRO	415 415	25.978 26.655	24.200 24.548	-1.983 -1.013	1.00	0.00	3A4
ATOM ATOM	2967	N	GLU	416	25.547	25.077	-2.937	1.00	0.00	3A4
ATOM	2968	CA	GLU	416	25.810	26.505	-2.951	1.00	0.00	3A4
MOTA	2969	СВ	GLU	416	27.244	26.943	-3.438	1.00	0.00	3A4 3A4
MOTA	2970	CG	GLU	416	28.338	26.841	-2.361	1.00	0.00	3A4
ATOM ATOM	2971 2972	CD OE1	GLU	416 416	29.636 29.584	27.541 28.756	-2.784 -3.114	1.00	0.00	3A4
• ATOM	2973		GLU	416	30.704	26.872	-2.759	1.00	0.00	3A4
ATOM	2974	c	GLU	416	24.818	27.126	-3.902	1.00	0.00	3A4
MOTA	2975	0	GLU	416	24.357	26.500	-4.855	1.00	0.00	3A4 3A4
MOTA	2976	N	ARG	417	24.555	28.429 29.448	-3.633 -4.465	1.00	0.00	3A4
ATOM ATOM	2977 2978	CA CB	ARG ARG	417 417	23.940 22.623	29.440	-5.229	1.00	0.00	3A4
ATOM	2979	CG	ARG	417	21.420	28.657	-4.370	1.00	0.00	3A4
ATOM	2980	CD	ARG	417	20.160	28.317	-5.191	1.00	0.00	3A4
MOTA	2981	NE	ARG	417	19.654	29.550	-5.895	1.00	0.00	3A4

	ATOM	2982	CZ	ARG	417	18.836	30.485	-5.308	1.00	0.00	3A4
•	ATOM	2983	NH1		417	18.453	31.575	-6.033	1.00	0.00	3A4 3A4
	ATOM	2984	NH2 C	ARG ARG	417 417	18.396 23.675	30.357 30.614	-4.021 -3.534	1.00	0.00	3A4
	ATOM ATOM	2985 2986	Ö	ARG	417	23.277	31.695	-3.966	1.00	0.00	3A4
	ATOM	2987	N	PHE	418	23.883	30.380	-2.207	1.00	0.00	. 3A4
	ATOM	2988	CA	PHE	418	23.598	31.253	-1.087	1.00	0.00	3A4
	MOTA	2989	CB	PHE	418	22.842	30.493	0.064	1.00	0.00	3A4
	ATOM	2990	CG	PHE	418	23.400	29.109	0.354 1.245	1.00	0.00	3A4 3A4
	ATOM ATOM	2991 2992	CD1		418 418	24.479 22.845	28.931 27.967	-0.262	1.00	0.00	3A4
	ATOM	2993		PHE	418	25.002	27.653	1.496	1.00	0.00	3A4
	MOTA	2994		PHE	418	23.361	26.688	-0.007	1.00	0.00	3A4
	MOTA	2995	CZ	PHE	418	24.442	26.532	0.869	1.00	0.00	3A4
	ATOM	2996	C	PHE	418	24.891 25.978	31.865 31.337	-0.589 -0.822	1.00	0.00	3A4 3A4
	ATOM ATOM	2997 2998	O N	PHE	418 419	24.764	33.010	0.130	1.00	0.00	3A4
	ATOM	2999	CA	SER	419	25.850	33.749	0.742	1.00	0.00	3A4
	ATOM	3000	СВ	SER	419	26.168	35.084	0.003	1.00	0.00	3A4
	ATOM	3001	OG	SER	419	26.610	34.824	-1.323	1.00	0.00	3A4
	ATOM	3002	C	SER	419	25.419	34.042 33.869	2.158 2.516	1.00	0.00	3A4 3A4
	ATOM ATOM	3003 3004	O N	SER Lys	419 420	24.254 26.380	34.507	2.995	1.00	0.00	3A4
	ATOM	3005	CA	LYS	420	26.162	34.853	4.383	1.00	0.00	3A4
	ATOM	3006	СВ	LYS	420	26.449	33.660	5.338	1.00	0.00	3A4
	ATOM	3007	CG	LYS	420	26.041	33.882	6.806	1.00	0.00	3A4
	MOTA	3008	CD	LYS	420	25.973 27.316	32.611 31.947	7.673 8.025	1.00	0.00	3A4 3A4
	ATOM ATOM	3009 3010	CE NZ	LYS LYS	420 420	27.897	31.201	6.884	1.00	0.00	3A4
	ATOM	3011	c	LYS	420	27.070	36.024	4.656	1.00	0.00	3A4
	ATOM	3012	0	LYS	420	28.205	36.070	4.182	1.00	0.00	3A4
	ATOM.	3013	N	LYS	421	26.554	37.018	5.432 5.697	1.00	0.00	3A4 3A4
	MOTA MOTA	3014 3015	CA CB	LYS LYS	421 421	27.150 26.041	38.319 39.410	5.739	1.00	0.00	. 3A4
	ATOM .	3016	CG	LYS	421	26.518	40.872	5.751	1.00	0.00	3A4
	MOTA	3017	CD	LYS	421,	25.360	41.868	5.629	1.00	0.00	3A4
	ATOM	3018	CE	LYS	421	25.821	43.332	5.619	1.00	0.00	3A4 3A4
	ATOM ATOM	3019 3020	NZ C	LYS LYS	421 421	24.664 27.940	44.251 38.313	5.492 6.992	1.00	0.00	3A4
	ATOM	3021	Ö	LYS	421	28.871	39.099	7.165	1.00	0.00	3A4
	MOTA	3022	N	ASN	422	27.572	37.398	7.933	1.00	0.00	3A4
	MOTA	3023	CA	ASN	422	28.154	37.237	9.255	1.00	0.00	3A4 3A4
	MOTA	3024 3025	CB CG	ASN ASN	422 422	27.020 27.499	37.047 37.210	10.319 11.776	1.00	0.00	3A4 3A4
	ATOM ATOM	3025		ASN	422	27.456	36.260	12.556	1.00	0.00	3A4
	ATOM	3027		ASN	422	27.964	38.434	12.149	1.00	0.00	3A4
		3028	С	ASN	422	29.107	36.052	9.222	1.00	0.00	3A4
	MOTA	3029	0	ASN	422	29.035	35.203	8.335 10.220	1.00	0.00	3A4 . 3A4
	MOTA MOTA	3030 . 3031	N CA	LYS LYS	423 423	30.033 31.052	35.989 34.968	10.220	1.00	0.00	3A4
	ATOM	3032	СВ	LYS	423	32.450	35.576	10.704	1.00	0.00	3A4
	MOTA	3033	CG	LYS	423	33.030	36.450	9.575	1.00	0.00	3A4
	ATOM	3034	CD	LYS	423	33.266	35.769	8.209	1.00	0.00	3A4 3A4
	ATOM .	3035	CE	LYS	423 423	34.431 34.107	34.762 33.470	8.142 8.794	1.00	0.00	3A4
	MOTA MOTA	3036 3037	NZ C	LYS LYS	423	30.631	34.032	11.491	1.00	0.00	3A4
	ATOM	3038	ŏ	LYS	423	30.939	34.245	12.663	1.00	0.00	3A4
	MOTA	3039	N	ASP	424	29.907	32.953	11.101	1.00	0.00	3A4
	ATOM	3040	CA	ASP	424	29.457	31.893	11.976 12.651	1.00	0.00	3A4 3A4
	MOTA MOTA	3041 3042	CB CG	ASP ASP	424 424	28.060 26.909	32.147 32.519	11.687	1.00	0.00	3A4
	ATOM	3043		ASP	424	25.944	31.714	11.589	1.00	0.00	3A4
	ATOM	3044		ASP	424	26.973	33.604	11.051	1.00	0.00	3A4
	ATOM	3045	С	ASP	424	29.495	30.648	11.123	1.00	0.00	3A4
	ATOM	3046	0	ASP	424 425	28.470 30.728	30.043 30.251	10.811 10.724	1.00	0.00	3A4 3A4
	MOTA MOTA	3047 3048	N CA	ASN ASN	425 425	30.728	29.112	9.872	1.00	0.00	3A4
	ATOM	3049	CB	ASN	425	30.910	29.449	8.339	1.00	0.00	3A4
	MOTA	3050	CG	ASN	425	31.718	30.701	7.912	1.00	0.00	3A4
	MOTA	3051		ASN	425	32.894	30.588	7.570	1.00	0.00	3A4 3A4
	MOTA MOTA	3052 3053	ND2 C	asn Asn	425 425	31.085 32.363	31.907 28.587	7.916 10.270	1.00	0.00	3A4
		2022	-	23 W LT		32.303	,		•		- · - -

ATOM	3054	0	ASN	425	33.092	28.033	9.449	1.00	0.00	3A4
ATOM	3055	N	ILE	426	32.734	28.773	11.570	1.00	0.00	3A4
MOTA	3056	CA	ILE	426	34.043	28.493	12.137	1.00	0.00	3A4
MOTA	3057	СВ	ILE	426	34.648	29.716	12.854	1.00	0.00	3A4
MOTA	3058		ILE	426	36.105	29.402	13.297	1.00	0.00	3A4
MOTA	3059		ILE	426	34.591	30.966	11.928	1.00	0.00	3A4 3A4
ATOM	3060	CD	ILE	426	35.100 33.870	32.260 27.289	12.569 13.047	1.00	0.00	3A4
MOTA	3061	C	ILE	426 426	34.107	26.155	12.633	1.00	0.00	3A4
MOTA MOTA	3062 3063	O N	ILE ASP	427	33.447	27.532	14.315	1.00	0.00	3A4
ATOM	3064	CA	ASP	427	33.204	26.537	15.348	1.00	0.00	3A4
ATOM	3065	СВ	ASP	427	34.320	26.450	16.444	1.00	0.00	3A4
MOTA	3066	CG	ASP	427	35.639	25.963	15.828	1.00	0.00	3A4
MOTA	3067	OD1	ASP	427	35.660	24.821	15.293	1.00	0.00	3A4
MOTA	3068	OD2	ASP	427	36.643	26.722	15.888	1.00	0.00	3A4
ATOM	3069	С	ASP	427	31.841	26.813	15.973	1.00	0.00	3A4
MOTA	3070	0	ASP	427	31.098	25.842	16.103	1.00	0.00	3A4 3A4
ATOM	3071	N	PRO	428	31.390	28.043 28.361	16.369 16.637	1.00	0.00	3A4
ATOM	3072	CA	PRO	428 428	29.983 32.272	29.141	16.778	1.00	0.00	3A4
ATOM ATOM	3073 3074	CD CB	PRO PRO	428	30.041	29.613	17.539	1.00	0.00	3A4
ATOM	3075	CG	PRO	428	31.359	30.308	17.172	1.00	0.00	3A4
ATOM	3076	c	PRO	428	29.245	28.611	15.321	1.00	0.00	3A4
ATOM	3077	0	PRO	428	29.471	29.640	14.687	1.00	0.00	3A4
ATOM .	3078	N	TYR	429	28.385	27.650	14.899	1.00	0.00	3A4
ATOM	3079	CA	TYR	429	27.755	27.649	13.596	1.00	0.00	3A4
MOTA	3080	CB	TYR	429	28.727	27.191	12.437	1.00	0.00	3A4
ATOM	3081	CG	TYR	429	29.325	25.786	12.428	1.00	0.00	3A4 3A4
ATOM	3082		TYR	429	29.871	25.334	11.208	1.00	0.00	3A4
ATOM	3083		TYR TYR	429	29.371 30.418	24.901 24.050	13.532 11.078	1.00	0.00	3A4
MOTA MOTA	3084 3085		TYR	429 429	29.917	23.615	13.410	1.00	0.00	3A4
ATOM	3086	CZ	TYR	129	30.437	23.186	12.181	1.00	0.00	3A4
ATOM	3087	ОН	TYR	429	30.972	21.885	12.055		0.00	3A4
ATOM	3088	С	TYR	429	26.500	26.805	13.683	1.00	0.00	3A4
ATOM	3089	0	TYR	429	25.984	26.542	14.769	1.00	0.00	3A4
ATOM	3090	N	ILE	430	26.004	26.339	12.499	1.00	0.00	3A4
ATOM	3091	CA		. 430	24.912	25.392	12.301	1.00	0.00	3A4
MOTA	3092	CB	ILE	430	23.953	25.845	11.196	1.00	0.00	3A4 3A4
ATOM	3093		ILE	430 430	23.323	27.171 26.004	11.680 9.800	1.00	0.00	3A4
ATOM ATOM	3094 3095	CG1	ILE	430	23.667	26.472	8.700	1.00	0.00	3A4
ATOM	3096	c	ILE	130	25.562	24.051	12.005		0.00	3A4
ATOM	3097	ō	ILE	430	26.789	23.977	12.016	1.00	0.00	3A4
ATOM	3098	N	TYR	431	24.773	22.951	11.760	1.00	0.00	3A4
ATOM	3099	CA	TYR	431	25.198	21.604	11.414	1.00	0.00	3A4
ATOM	3100	CB	TYR	431	26.437	21.470	10.410	1.00	0.00	3A4
ATOM	3101	CG	TYR	431	26.384	22.218	9.097	1.00	0.00	3A4
ATOM.	3102		TYR	431	25.749	21.647	7.983 8.894	1.00	0.00	3A4 3A4
ATOM	3103		TYR TYR	431	27.142 25.834	23.393 22.246	6.714	1.00	0.00	3A4
ATOM ATOM	3104 3105		TYR	431 431	27.212	24.010	7.638	1.00	0.00	3A4
ATOM	3106	CZ	TYR	431	26.551	23.437	6.544	1.00	0.00	3A4
ATOM	3107	ОН	TYR	431	26.632	24.036	5.267	1.00	0.00	3A4
ATOM	3108	С	TYR	431	25.647	20.889	12.688	1.00	0.00	3A4
ATOM	3109	0	TYR	431	26.635	21.285	13.303	1.00	0.00	3A4
MOTA	3110	N	THR	432	24.989	19.782	13.089	1.00	0.00	3A4
MOTA	3111	CA	THR	432	25.445	18.960	14.203	1.00	0.00	3A4
MOTA	3112	СВ	THR	432	24.381	18.938	15.316	1.00	0.00 0.00	3A4 3A4
ATOM	3113		THR	432	23.070	18.659 20.310	14.826 16.028	1.00	0.00	3A4
MOTA MOTA	3114 3115	CGZ	THR THR	432 432	24.399 25.810	17.558	13.781	1.00	0.00	3A4
ATOM	3116	ò	THR	432	25.565	16.648	14.576	1.00	0.00	3A4
ATOM	3117	N	PRO	433	26.389	17.234	12.610	1.00	0.00	3A4
ATOM	3118	CA	PRO	433	26.601	15.849	12.240	1.00	0.00	3A4
MOTA	3119	CD	PRO	433	27.173	18.101	11.724	1.00	0.00	3A4
MOTA	3120	ÇВ	PRO	433	26.947	15.918	10.740	1.00	0.00	3A4
ATOM	3121	CG	PRO	433	27.743	17.221	10.601	1.00	0.00	3A4
MOTA	3122	C	PRO	433	27.748	15.209	13.022	1.00	0.00	3A4 3A4
ATOM	3123	0	PRO	433	27.771 28.673	13.993 16.013	13.150 13.587	1.00	0.00 0.00	3A4
MOTA	3124	N CA	PHE -	434 434	28.673	15.548	14.382	1.00	0.00	3A4
ATOM	3125	CM	PHE	424	27.702	10.040	14.302			

ATOM	3126	СВ	PHE	434	31.108	16.257	13.997	1.00	0.00	3A4
ATOM	3127	CG	PHE	434	31.591	15.810	12.639	1.00	0.00	3A4
ATOM	3128	CD1		434	31.353	16.451	11.514	1.00	0.00	3A4
MOTA	3129	CD2	PHE	434	32.354	14.754	12.363	1.00	0.00	3A4
ATOM	3130	CEI		434	31.813	16.203	10.200	1.00	0.00	3A4
MOTA	3131	CE2		434	32.860	14.287	11.129	1.00	0.00	3A4 3A4
MOTA	3132	CZ	PHE	434	32.592	15.066	10.009	1.00	0.00	3A4
MOTA	3133	C	PHE	434	29.528	15.802	15.833	1.00	0.00	3A4
ATOM	3134	0	PHE	434	· 30.427 28.291	15.663 16.210	16.655 16.191	1.00	0.00	3A4
ATOM	3135	N CA	GLY GLY	435 435	27.923	16.495	17.561	1.00	0.00	3A4
ATOM ATOM	3136 3137	C	GLY	435	28.209	17.917	17.875	1.00	0.00	3A4
ATOM	3138	ŏ	GLY	435	28.305	18.719	16.943	1.00	0.00	3A4
ATOM	3139	N	SER	436	28.348	18.248	19.183	1.00	0.00	3A4
ATOM	3140	CA	SER	436	28.384	19.623	19.578	1.00	0.00	3A4
ATOM	3141	CB	SER	436	26.947	20.258	19.543	1.00	0.00	3A4
ATOM	3142	OG	SER	436	26.948	21.683	19.489	1.00	0.00	3A4 3A4
MOTA	3143	С	SER	436	29.197	19.916	20.769	1.00 1.00	0.00	3A4
MOTA	3144	0	SER	436	30.134 28.951	20.642 19.486	20.647	1.00	0.00	3A4
ATOM	3145	N	GLY GLY	437 437	29.675	19.961	23.144	1.00	0.00	3A4
ATOM	3146 3147	CA C	GLY	437	31.130	19.558	23.314	1.00	0.00	3A4
ATOM ATOM	3148	ŏ	GLY	437	31.959	19.487	22.402	1.00	0.00	3A4
ATOM	3149	N	PRO	438	31.502	19.228	24.529	1.00	0.00	3A4
ATOM	3150	CA	PRO	438	32.875	18.727	24.776	1.00	0.00	3A4
ATOM	3151	CD	PRO	438	30.927	19.742	25.770	1.00	0.00	3A4
MOTA	3152	CB	PRO		33.100	18.880	26.266	1.00	0.00	3A4
MOTA	3153	CG	PRO	438	31.706	19.063	26.880	1.00	0.00	3A4 3A4
MOTA	3154	С	PRO	438	33.099	17.295	24.317	1.00	0.00	3A4
MOTA	3155	0	PRO	438	34.230 32.033	16.824 16.608	24.348 23.850	1.00	0.00	3A4
MOTA	3156	N	ARG ARG	439 439	32.068	15.264	23.366	1.00	0.00	3A4
MOTA MOTA	3157 3158	CA CB	ARG	439	30.905	14.467	23.961	1.00	0.00	3A4
ATOM	3159	CG	ARG	439	30.793	14.766	25.461	1.00	0.00	3A4
ATOM	3160	CD	ARG	439	30.197	13.690	26.366	1.00	0.00	3A4
ATOM	3161	NE	ARG	439	30.391	14.136	27.786	1.00	0.00	3A4
MOTA	3162	CZ	ARG	439	30.091	13.354	28.866	1.00	0.00	3A4
MOTA	3163		ARG	439	30.342	13.836	30.116	1.00	0.00	3A4 3A4
ATOM	3164		ARG	439	29.553	12.109	28.713	1.00	0.00	3A4
ATOM	3165	C	ARG	439	31.980 31.776	15.221 14.165	21.890 21.309	1.00	0.00	3A4
MOTA	3166	0	ARG	439 440	32.201	16.364	21.200	1.00	0.00	3A4
ATOM	3167 3168	N CA	ASN	440	32.204	16.474	19.756	1.00	0.00	3A4
MOTA	3169	CB	ASN	440	32.625		19.354	1.00	0.00	3A4
ATOM	3170	CG	ASN	440	32.279	18.329	17.901	1.00	0.00	3A4
ATOM	3171	OD1	ΛSN	440	32.746	17.778	16.907	1.00	0.00	3A4
ATOM	3172	ND2	ASN	440	31.452	19.401	17.765	1.00	0.00	3A4
ATOM	3173	С	ASN	440	33.216	15.539	19.171	1.00	0.00	3A4 3A4
ATOM	3174	0	ASN	440.	34.241	15.285	19.807 17.974	1.00	0.00	3A4
ATOM	3175	И	CYS	441	32.950 33.782	14.993 14.009	17.328	1.00	0.00	3A4
MOTA	3176	CA	CYS	441 441	33.782	13.772	15.899	1.00	0.00	3A4
MOTA MOTA	3177 3178	CB SG	CYS	441	34.028	12.338	15.029	1.00	0.00	3A4
ATOM	3179	c	CYS	441	35.241	14.414	17.264	1.00	0.00	3A4
ATOM	3180	ō	CYS	441	35.564	15.528	16.866	1.00	0.00	3A4
ATOM	3181	N	ILE	442	-36.131	13.531	17.746	1.00	0.00	3A4
ATOM	3182	CA	ILE	442	37.556	13.799	17.790	1.00	0.00	3A4
MOTA	3183	СВ	ILE	442	38.223	12.944	18.848	1.00	0.00	3A4 3A4
ATOM	3184		ILE	442	38.388	11.476 13.570	18.448 19.391	1.00	0.00	3A4
ATOM	3185		ILE	442 442	39.528 39.336	14.819	20.250	1.00	0.00	3A4
MOTA MOTA	3186 3187	CD	ILE	442	38.181	13.605	16.408	1.00	0.00	3A4
ATOM	3188	ò	ILE	442	39.180	14.220	16.048		0.00	3A4
ATOM	3189	N	GLY	443	37.524	12.758	15.590		0.00	3A4
ATOM	3190	CA	GLY	443	37.942	12.408	14.266		0.00	3A4
ATOM	3191	С	GLY	443	37.399	13.252	13.158		0.00	3A4
ATOM	3192	0	GLY	443	37.591	12.902	12.001		0.00	3A4
MOTA	3193	N	MET	444	36.732	14.396	13.456			3A4 3A4
ATOM	3194	CA	MET	444	36.082	15.266	12.493 13.192			3A4
ATOM	3195	CB	MET	414 444	35.408 36.294	16.458 17.310	14.126			. 3A4
ATOM	3196 3197	CG SD	MET MET	444	35.375	18.583	15.041			3A4
MOTA	717/	30	1	***	55.5.5				_	

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MOTA	3198	CE	MET	444	36.695	18.911	16.244	1.00	0.00	3A4
MOTA	3199	С	MET	444	36.968	15.807	11.395	1.00	0.00	3A4
ATOM	3200	0	MET	444	36.570	15.844	10.236	1.00	0.00	3A4 3A4
ATOM	3201	N	ARG	445	38.230 39.211	16.170 16.708	11.727 10.801	1.00	0.00	3A4
ATOM ATOM	3202 3203	CA CB	ARG ARG	445 445	40.435	17.321	11.549	1.00	0.00	3A4
ATOM	3204	CG	ARG	445	40.058	18.332	12.647	1.00	0.00	3A4
ATOM	3205	CD	ARG	445	39.223	19.529	12.155	1.00	0.00	3A4
ATOM	3206	NE	ARG	445	38.880	20.389	13.341	1.00	0.00	3A4
ATOM	3207	CZ	ARG	445	37.901	21.351	13.313	1.00	0.00	3A4
MOTA	3208	NH1		445	37.643	22.071	14.443	1.00	0.00	3A4 3A4
ATOM	3209		ARG	445	37.171 39.695	21.600 15.651	12.186 9.828	1.00	0.00	3A4
ATOM ATOM	3210 3211	С 0	ARG ARG	445 445	39.790	15.886	8.628	1.00	0.00	3A4
ATOM	3212	N	PHE	446	39.920	14.418	10.335	1.00	0.00	3A4
ATOM	3213	CA	PHE	446	40.293	13.256	9.549	1.00	0.00	3A4
ATOM	3214	СВ	PHE	446	40.683	12.116	10.501	1.00	0.00	3A4
MOTA	3215	CG	PHE	446	41.549	11.008	9.982	1.00	0.00	3A4
ATOM	3216		PHE	446	42.800	11.292	9.403	1.00	0.00	3A4 3A4
ATOM	3217 3218	CD2	PHE	446 446	41.248 43.749	9.684 10.278	10.350 9.241	1.00	0.00	3A4
ATOM ATOM	3219		PHE	446	42.210	8.678	10.222	1.00	0.00	3A4
ATOM	3220	cz	PHE	446	43.469	8.983	9.689	1.00	0.00	3A4
ATOM	3221	С	PHE	446	39.172	12.804	8.647	1.00	0.00	3A4
MOTA	3222	0	PHE	446	39.384	12.508	7.480	1.00	0.00	3A4
MOTA	3223	N	ALA	447	. 37.921	12.812	9.148	1.00	0.00	3A4
MOTA	3224	CA	ALA	447	36.738	12.472	8.393 9.272	1.00	0.00	3A4 3A4
ATOM ATOM	3225 3226	CB C	ALA ALA	447 447 .	35.499 36.489	12.464 13.392	7.228		0.00	3A4
ATOM	3227	o	ALA	447	36.216	12.950	6.120	1.00	0.00	3A4
ATOM	3228	N	LEU	448	36.656	14.715	7.427	1.00	0.00	3A4
ATOM	3229	CA	LEU	448	36.469	15.704	6.386	1.00	0.00	3A4
MOTA	3230	CB	LEU	448	36.399	17.124	6.962	1.00	0.00	3A4
ATOM	3231		LEU	448	35.089	17.408	7.731	1.00	0.00	3A4
ATOM	3232	CD1		448	35.223 33.842	18.721 17.445	8.515 6.826	1.00	0.00	3A4 3A4
ATOM ATOM	3233 3234	CD2	LEU	448 448	37.561	15.661	5.351	1.00	0.00	3A4
ATOM	3235	ō	LEU	448	37.299	15.865	4.175	1.00	0.00	3A4
ATOM	3236	N	MET	449	38.806	15.319	5.746	1.00	0.00	3A4
ATOM	3237	CA	MET	449	39.935	15.178	4.853	1.00	0.00	3A4
ATOM	3238	CB	MET	449	41.269	15.033	5.617	1.00	0.00	3A4
ATOM	3239	CG	MET	449	41.841	16.358	6.130	1.00	0.00	3A4 3A4
ATOM ATOM	3240 3241	SD CE	MET MET	449 449	43.382	16.135 17.904	7.075 7.332	1.00	0.00	3A4
ATOM	3242	C	MET	449	39.772	13.984	3.951	1.00	0.00	3A4
ATOM	3243	ŏ	MET	449	39.956	14.095	2.746	1.00	0.00	3A4
ATOM	3244	N	ASN	450	39.332	12.829	4.502	1.00	0.00	3A4
MOTA	3245	CA	ASN	450	39.098	11.625	3.740	1.00	0.00	3A4
ATOM	3246	CB	ASŅ	450	38.915	10.385	4.623	1.00	0.00	3A4. 3A4
ATOM	3247	CG	ASN	450	37.685	10.130 10.268	5.531 5.191	1.00	0.00	3A4
MOTA MOTA	3248 3249	ND2	ASN	450 450	36.512 37.990	9.606	6.751	1.00	0.00	3A4
ATOM	3250	C	ASN	450	37.976	11.740	2.750	1.00	0.00	3A4
ATOM	3251	ō	ASN	450	38.095	11.281	1.623	1.00	0.00	3A4
ATOM	3252	N	MET	451	36.874	12.422	3.129	1.00	0.00	3A4
ATOM	3253	CA	MET	451	35.744	12.687	2.267	1.00	0.00	3A4
MOTA	3254	CB	MET	451	34.596	13.445	3.021	1.00	0.00	3A4 3A4
ATOM	3255	CG	MET	451 451	33.788 32.502	12.610 13.565	4.010 4.863	1.00	0.00	3A4
MOTA MOTA	3256 3257	SD CE	MET MET	451 451	33.061	13.383	6.570	1.00	0.00	3A4
ATOM	3258	c	MET	451	36.081	13.580	1.106	1.00	0.00	3A4
ATOM	3259	ō	MET	451	35.746	13.314	-0.041	1.00	0.00	3A4
ATOM	3260	N	LYS	452	36.821	14.667	1.389	1.00	0.00	3A4
ATOM	3261	CA	LYS	452	37.237	15.652	0.424	1.00	0.00	3A4
ATOM	3262	CB	LYS	452	37.854	16.860	1.154	1.00	0.00	3A4 3A4
MOTA MOTA	3263 3264	CG CD	LYS LYS	452 452	37.750 38.346	18.227 19.380	0.470 1.301	1.00	0.00	3A4
ATOM	3265	CE	LYS	452	38.006	19.391	2.808	1.00	0.00	3A4
ATOM	3266	NZ	LYS	452	36.543	19.337	3.053	1.00	0.00	3A4
ATOM	3267	С	LYS	452	38.228	15.110	-0.572	1.00	0.00	3A4
ATOM	3268	0	LYS	452	38.108	15.335	-1.769	1.00	0.00	3A4
ATOM	3269	N	LEU	453	39.207	14.309	-0.102	1.00	0.00	3A4

ATOM	3270	CA	LEU	453	40.212	13.676	-0.927	1.00	0.00	3A4
ATOM	3271	СВ	LEU	453	41.342	13.071	-0.061	1.00	0.00	3A4
ATOM	3272	CG	LEU	453	42.298	14.219	0.403	1.00	0.00	3A4
ATOM	3273	CD1	LEU	453	43.187	13.854	1.595	1.00	0.00	3A4
MOTA	3274	CD2	LEU	453	43.191	14.764	-0.734	1.00	0.00	3A4
ATOM	3275	С	LEU	453	39.621	12.644	-1.845	1.00	0.00	3A4
ATOM	3276	0	LEU	453	39.939	12.613	-3.026	1.00	0.00	3A4
ATOM	3277	N	λLA	454	38.662	11.829	-1.353	1.00	0.00	3A4
MOTA	3278	CA	ALA	454	37.935	10.847	-2.131	1.00	0.00	3A4
ATOM	3279	СВ	ALA	454	37.013	9.992	-1.240	1.00	0.00	374
ATOM	3280	С	ALA	454	37.093	11.464	-3.225	1.00	0.00	3A4
MOTA	3281	0	ALA	454	37.181	11.055	-4.371	1.00	0.00	3A4
ATOM	3282	N	LEU	455	36.307	12.514	-2.904	1.00	0.00	3A4
ATOM	3283	CA	LEU	455	35.457	13.201	-3.852	1.00	0.00	3A4
ATOM	3284	CB	LEU	455	34.480	14.157	-3.157	1.00	0.00	3A4
MOTA	3285	CG	LEU	455	33.366	13.559	-2.303	1.00	0.00	3A4
ATOM	3286	CD1	LEU	455	32.576	14.761	-1.760	1.00	0.00	3A4
MOTA	3287	CD2	LEU	455	32.474	12.556	-3.064	1.00	0.00	3A4
MOTA	3288	C	LEU	455	36.203	14.018	-4.886	1.00	0.00	3A4
MOTA	3289	0	LEU	455	35.736	14.147	-6.009	1.00	0.00	3A4
MOTA	3290	N	ILE	456	37.412	14.540	-4.555	1.00	0.00	3A4
ATOM	3291	CA	ILE	456	38.284	15.264	-5.474	1.00	0.00	3A4
MOTA	3292	CB	ILE	456	39.413	16.061	-4.749	1.00	0.00	3A4
MOTA	3293	CG2	ILE	456	40.832	16.074	-5.412	1.00	0.00	3A4
MOTA	3294	CGI	ILE	456	39.003	17.537	-4.565	1.00	0.00	3A4
ATOM	3295	CD	ILE	456	38.041	17.823	-3.423	1.00	0.00	3A4
ATOM	3296	С	ILE	456	38.894	14.318	-6.496	1.00	0.00	3A4
MOTA	3297	0	ILE	456	39.099	14.677	-7.647	1.00	0.00	3A4
MOTA	3298	N	ARG	457	39.181	13.066	-6.083	1.00	0.00	3A4
MOTA	3299	CA	ARG	457	39.859	12.081	-6.895	1.00	0.00	3A4
ATOM	3300	СВ	ARG	457	40.758	11.186	-6.025	1.00	0.00	3A4
ATOM	3301	CG	ARG	457	41.905	12.005	-5.430	1.00	0.00	3A4
ATOM	3302	CD	ARG	457	42.735	11.300	-4.341	1.00	0.00	3A4
ATOM	3303	NE	ARG	457	43.559	12.343	-3.632	1.00	0.00	3A4
ATOM	3304	CZ	ARG	457	44.624	12.985	-4.211	1.00	0.00	3A4 3A4
ATOM	3305		ARG	457	45.148	14.087	-3.601	1.00	0.00	3A4
ATOM	3306		ARG	457	45.174 38.924	12.558	-5.385 -7.722	1.00	0.00	3A4
ATOM	3307 3308	C	ARG	457 457	39.246	11.235 10.873	-8.848	1.00	0.00	3A4
ATOM ATOM	3309	O N	ARG VAL	458	37.713	10.918	-7.207	1.00	0.00	3A4
ATOM	3310	CA	VAL	458	36.711	10.092	-7.872	1.00	0.00	3A4
ATOM	3311	CB	VAL	458	35.631	9.662	-6.887	1.00	0.00	3A4
ATOM	3312		VAL	458	34.290	9.133	-7.471	1.00	0.00	3A4
ATOM	3313		VAL	458	36.253	8.556	-6.006	1.00	0.00	3A4
ATOM	3314	c	VAL	458	36.101	10.798	-9.063	1.00	0.00	3A4
ATOM	3315	ŏ.	VAL	458	36.040		-10.146	1.00	0.00	3A4
ATOM	3316	N	LEU	459	35.685	12.071	-8.900	1.00	0.00	3A4
ATOM	3317	CA	LEU	459	34.979	12.841	-9.906	1.00	0.00	3A4
ATOM	3318	СВ	LEU	459	34.354	14.096	-9.255	1.00	0.00	3A4
ATOM	3319	CG	LEU	459	33.225	13.778	-8.265	1.00	0.00	3A4
ATOM	3320		LEU	459	32.786	15.037	-7.500	1.00	0.00	3A4
ATOM	3321		LEU	459	32.041	13.132	-8.991	1.00	0.00	3A4
ATOM	3322	С	LEU	459	35.826		-11.060	1.00	0.00	3A4
MOTA	3323	0	LEU	459	35.319	13.601	-12.136	1.00	0.00	3A4
MOTA	3324	N	GLN	460	37.158	13.371	-10.874	1.00	0.00	3A4
MOTA	3325	CA	GLN	460	38.070	13.748	-11.927	1.00	0.00	3A4
MOTA	3326	CB	GLN	460	39.373	14.365	-11.376	1.00	0.00	3A4
MOTA	3327	CG	GLN	460	39.106	15.740	-10.736	1.00	0.00	3A4
MOTA	3328	CD	GLN	460	40.408	16.286	-10.160	1.00	0.00	3A4
ATOM	3329	OE1	GLN	460	41.430	15.608	-10.237	1.00	0.00	3A4
ATOM	3330	NE2	GLN	460	40.380	17.515	-9.575	1.00	0.00	3A4
MOTA	3331	С	GLN	460	38.365	12.562	-12.815	1.00	0.00	3A4
MOTA	3332	0	GLN	460	38.683		-13.990	1.00	0.00	3A4
ATOM	3333	N	ASN	461	38.258		-12.266	1.00	0.00	3A4
ATOM	3334	CA	ASN	461	38.598		-12.957	1.00	0.00	3A4
MOTA	3335	CB	ASN	461	39.328		-12.018	1.00	0.00	3A4
ATOM	3336	CG	ASN	461	40.725		-11.730	1.00	0.00	3A4
MOTA	3337	OD1		461	41.364		-12.617	1.00	0.00	3A4
ATOM	3338	ND2		461	41.239		-10.482	1.00	0.00	3A4
ATOM	3339	С	ASN	461	37.402		-13.562	1.00	0.00	3A4
ATOM	3340	0	ASN	461	37.588		-14.451	1.00	0.00	3A4
MOTA	3341	N	PHE	462	36.167	9.725	-13.107	1.00	0.00	3A4

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ATOM	3342	CA	PHE	462	34.983	8.975	-13.533	1.00	0.00	3A4
ATOM	3343	CB	PHE	462	34.346		-12.354	1.00	0.00	3A4
ATOM'	3344	CG	PHE	462	35.274	7.073	-11.873	1.00	0.00	3A4
MOTA	3345	CD1		462	35.686		-12.745	1.00	0.00	3A4 3A4
ATOM	3346	CD2		462	35.718 36.530		-10.540 -12.307	1.00	0.00	3A4
ATOM ATOM	3347 3348	CE1		462 462	36.561		-10.089	1.00	0.00	3A4
ATOM	3349	CZ	PHE	462	36.972		-10.978	1.00	0.00	3A4
ATOM	3350	C	PHE	462	33.836	9.848	-14.135	1.00	0.00	3A4
ATOM .	3351	0	PHE	462	33.734		-13.828	1.00	0.00	3A4
ATOM	3352	N	SER	463	32.784 31.446		-15.007 -15.542	1.00	0.00	3A4 3A4
ATOM ATOM	3353 3354	CA CB	SER	463 463	31.440		-17.094	1.00	0.00	3A4
ATOM	3355	OG	SER	463	32.293		-17.565	1.00	0.00	3A4
ATOM	3356	С	SER	463	30.513		-15.014	1.00	0.00	3A4
MOTA	3357	0	SER	463	30.243		-15.673	1.00	0.00	3A4 3A4
ATOM	3358	N	PHE	464 464	30.012 29.251		-13.767 -13.078	1.00	0.00	3A4
MOTA MOTA	3359 3360	CA CB	PHE	464	29.689		-11.603	1.00	0.00	3A4
ATOM .	3361	ĊG	PHE	464	29.600		-10.565	1.00	0.00	3A4
ATOM	3362	CD1		464	30.780	9.102	-9.999	1.00	0.00	3A4
ATOM	3363	CD2		464	28.364	8.952 9.958	-9.990 -8.891	1.00 1.00	0.00 0.00	3A4 3A4
ATOM	3364 3365	CE1		464 464	30.727 28.310	9.832	-8.899	1.00	0.00	3A4
ATOM ATOM	3366	CZ	PHE	464	29.493	10.333	-8.347	1.00	0.00	3A4
ATOM	3367	Č	PHE	464	27.768		-13.199	1.00	0.00	3A4
ATOM	3368	0	PHE	464	27.238		-13.175	1.00	0.00	3A4 3A4
ATOM	3369	N	LYS	465	27.076 25.646		-13.331 -13.439	1.00	0.00	3A4
ATOM ATOM	3370 3371	CA CB	LYS	465 465	25.040		-14.891	1.00	0.00	3A4
ATOM	3372	CG	LYS	465	25.553		-15.915	1.00	0.00	3A4
ATOM	3373	CD	LYS	465	25.067		-17.333	1.00	0.00	3A4
MOTA	3374	CE	LYS	465	25.438		-18.374	1.00	0.00	3A4 3A4
ATOM	3375	NZ	LYS	465 465	26.910 25.212		-18.512 -12.507	1.00	0.00	3A4
ATOM ATOM	3376 3377	C O	LYS	465	25.982		-12.254	1.00	0.00	3A4
ATOM	3378	N	PRO	466	23.983	5.622	-11.985	1.00	0.00	3A4
ATOM	3379	CA	PRO	466	23.422		-11.249	1.00	0.00	3A4
MOTA	3380	CD	PRO	466	23.090 22.300		-11.993 -10.405	1.00 1.00	0.00	3A4 3A4
ATOM ATOM	3381 3382	CB CG	PRO PRO	466 466	21.827		-11.228	1.00	0.00	3A4
ATOM	3383	c	PRO	466	22.906	3.470	-12.228	1.00	0.00	3A4
ATOM	3384	0	PRO	466	22.333		-13.264	1.00	0.00	3A4
ATOM	3385	N	CYS	467	23.088 22.624		-11.890 -12.667	1.00 1.00	0.00	3A4 3A4
ATOM ATOM	3386 3387	CA CB	CYS	467 467	23.617		-12.501	1.00	0.00	3A4
ATOM	3388	SG	CYS	467	23.434		-13.674	1.00	0.00	3A4
ATOM	3389	С	CYS	467	21.212		-12.220	1.00	0.00	3A4
ATOM.	3390	0	CYS	467	20,555		-12.834 -11.130	1.00	0.00 0.00	3A4 3A4
ATOM ATOM	3391 3392	N CA	LYS LYS	468 468	20.726 19.389		-10.573	1.00	0.00	3A4
ATOM	3393	СВ	LYS	468	19.406	1.410		1.00	0.00	3A4
ATOM	3394	CG	LYS	468	20.290	0.367		1.00	0.00	3A4
MOTA	3395	CD	LYS	468	20.136	0.413		1.00	0.00	3A4 3A4
MOTA MOTA	3396 3397	CE NZ	LYS LYS	468 468	21.077 20.807	-0.534 -0.485		1.00	0.00	3A4
MOTA	3398	c	LYS	468	18.586	2.429	-11.148	1.00	0.00	3A4
MOTA	3399	0	LYS	468	19.145		-11.548	1.00	0.00	3A4
MOTA	3400	N	GLU	469	17.238		-11.203	1.00	0.00	3A4 3A4
ATOM	3401	CA CB	GLU	469 469	16.301 15.428		-11.832 -12.905	1.00	0.00	3A4
MOTA MOTA	3402 3403	CG	GLU	469	16.234		-14.000	1.00	0.00	3A4
ATOM	3404	CD	GLU	469	17.104	2.712	-14.780	1.00	0.00	3A4
MOTA	3405		GLU	469	16.530		-15.407	1.00	0.00	3A4
ATOM	3406		GLU	469	18.355		-14.761 -10.753	1.00	0.00	3A4 3A4
MOTA MOTA	3407 3408	C O	GT. GT.	469 469	15.433 15.841	3.792		1.00	0.00	3A4
ATOM	3408	N	THR	470	14.183		-11.133	1.00	0.00	3A4
ATOM	3410	CA	THR	470	13.125		-10.289	1.00	0.00	3A4
MOTA	3411	СВ	THR	470	12.400		-10.998	1.00	0.00	3A4 3A4
ATOM	3412		THR	470 470	11.519 11.657		/ -10.138 / -12.286	1.00	0.00	3A4
MOTA	3413	CGZ	THR	770	11.037	3.421	12.200			

ATOM	3414	С	THR	470	12.198	3.578	-9.882	1.00	0.00	3A4
ATOM	3415	ō	THR	470	11.456	3.677	-8.906	1.00	0.00	3A4
ATOM	3416	N	GLN	471	12.279	2.447 -		1.00	0.00	3A4
MOTA	3417	CA	GLN	471	11.670	1.158 -		1.00	0.00	3A4 3A4
ATOM	3418	CB	GLN	471	10.997		-11.656	1.00	0.00	3A4
ATOM	3419	CG	GLN	471	11.811		-12.967	1.00	0.00	3A4
MOTA	3420	CD	GLN	471	10.976 10.763	-1.106	-14.119 -14.193	1.00	0.00	3A4
MOTA	3421	OE1		471 471	10.783		-15.035	1.00	0.00	3A4
ATOM	3422	NE2	gln Gln	471	12.773	0.276	-9.839	1.00	0.00	3A4
ATOM ATOM	3423 3424	ò	GLN	471	13.605	-0.249		1.00	0.00	3A4
ATOM	3425	N	ILE	472	12.809	0.178	-8.475	1.00	0.00	3A4
ATOM	3426	CA	ILE	472	13.847	-0.369	-7.600	1.00	0.00	3A4
ATOM	3427	СВ	ILE	472	14.451	-1.737	-7.993	1.00	0.00	3A4
ATOM	3428	CG2	ILE	472	15.447	-2.232	-6.907	1.00	0.00	3A4
ATOM	3429	CG1	ILE	472	13.359	-2.820	-8.240	1.00	0.00	3A4 3A4
MOTA	3430	CD	ILE	472	12.440	-3.129	-7.050	1.00	0.00	3A4 3A4
ATOM	3431	С	ILE	472	14.926	0.710	-7.400 -8.188	1.00	0.00	3A4
ATOM	3432	0	ILE	472	15.870	0.760 1.594	-6.373	1.00	0.00	3A4
ATOM	3433	N	PRO	473 473	14.837 15.865	2.553	-5.978	1.00	0.00	3A4
MOTA	3434	CA CD	PRO PRO	473	13.607	1.778	-5.600	1.00	0.00	3A4
ATOM ATOM	3435 3436	CB	PRO	473	15.047	3.657	-5.263	1.00	0.00	3A4
ATOM	3437	CG	PRO	473	13.885	2.910	-4.607	1.00	0.00	3A4
ATOM	3438	c	PRO	473	16.926	1.936	-5.117	1.00	0.00	3A4
ATOM	3439	ō	PRO	473	17.147	0.726	-5.098	1.00	0.00	3A4
MOTA	3440	N	LEU	474	17.606	2.821	-4.384	1.00	0.00	3A4
MOTA	3441	CA	LEU	474	18.692	2.518	-3.506	1.00	0.00	3A4 3A4
ATOM	3442	CB	LEU	474	19.658	3.718	-3.467	1.00	0.00 0.00	3A4 3A4
MOTA	3443	CG	LEU	474	20.935	3.548	-2.623 -3.503	1.00	0.00	3A4
MOTA	3444		LEU	474	22.187 20.962	3.637 4.569	-1.472	1.00	0.00	3A4
MOTA	3445		LEU	474 474	18.157	2.198	-2.136	1.00	0.00	3A4
ATOM	3446 3447	С О	LEU LEU	474	17.397	2.966	-1.547	1.00	0.00	3A4
ATOM ATOM	3448	N	LYS	475	18.561	1.016	-1.612	1.00	0.00	3A4
ATOM	3449	CA	LYS	475	18.133	0.502	-0.330	1.00	0.00	3A4
ATOM	3450	СВ	LYS	475	18.199	-1.049	-0.249	1.00	0.00	3A4
ATOM	3451	CG	LYS	475	17.520	-1.656	0.999	1.00	0.00	3A4
ATOM	3452	CD	LYS	475	17.579	-3.189	1.074	1.00	0.00	3A4 3A4
MOTA	3453	CE	LYS	475	18.981	-3.776	1.311	1.00	0.00 0.00	3A4
ATOM	3454	NZ	LYS	475	19.572	-3.282 1.086	2.580 0.775	1.00	0.00	3A4
ATOM	3455	C	LYS	475 475	18.961 20.173	0.909	0.825	1.00	0.00	3A4
ATOM	3456 3457	O N	LYS LEU	476	18.276	1.798	1.695	1.00	0.00	. 3A4
ATOM ATOM	3458	CA	LEU	476	18.860	2.419	2.855	1.00	0.00	3A4
ATOM	3459		LEU	476	18.422	3.903	3.070	1.00	0.00	3A4
ATOM	3460	CG	·LEU	476	16.930	4.243	3.360	1.00	0.00	-3A4
ATOM	3461	CD1	LEU	476	16.813	5.725	3.764	1.00	0.00	3A4
MOTA	3462	CD2	LEU	476.	15.956	3.930	2.201	1.00	0.00	3A4 3A4
ATOM	3463	C	LEU	476	18.580	1.579	4.038	1.00	0.00	3A4
MOTA	3464	0	LEU	476	17.524	0.970 1.495	4.149 4.973	1.00	0.00	3A4
ATOM	3465	N	SER	477	19.543 19.480	0.545	6.040	1.00	0.00	3A4
MOTA	3466 3467	CA	SER	477 477	20.807	-0.220	6.343	1.00	0.00	3A4
ATOM ATOM	3468	CB OG	SER SER	477	20.584	-1.554	6.795	1.00	0.00	3A4
ATOM	3469	c	SER	477	18.826	1.150	7.228	1.00	0.00	3A4
ATOM	3470	ŏ	SER	477	18.936	2.334	7.525	1.00	0.00	3A4
ATOM	3471	N	LEU	478	18.068	0.282	7.917	1.00	0.00	3A4
ATOM	3472	CA	LEU	478	17.386	0.588		1.00	0.00	3A4
ATOM	3473	CB	LEU	478	16.072	-0.245		1.00		3A4 3A4
ATOM	3474	CG	LEU	478	15.314	-0.208		1.00		3A4
MOTA	3475		LEU	478	14.954	1.206 -1.098		1.00		3A4
ATOM	3476		LEU	478	14.057 18.338	0.280		1.00		3A4
ATOM	3477	C	LEU	478 478	18.566	-0.855				3A4
MOTA MOTA	3478 3479	N	LEU GLY		18.982	1.308		1.00		3A4
ATOM	3480	CA	GLY		19.983					3A4
ATOM	3481	c	GLY		19.558			1.00		384
ATOM	3482	ō	GLY		19.405	0.936				3A4
MOTA	3483	N	GLY		19.416					3A4
ATOM	3484	CA	GLY		19.205					3A4 3A4
MOTA	3485	С	GLY	480	20.442	4.355	14.943	1.00	0.00	JA4

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ATOM	3486	0	GLY	480	20.430	5.574	14.961	1.00	0.00	3A4
ATOM	3487	N	LEU	481	21.566	3.643	15.196	1.00	0.00	3A4
ATOM	3488	CA	LEU	481	22.833	4.218	15.597	1.00	0.00	3A4
MOTA	3489	CB	LEU	481	23.634	3.303	16.586	1.00	0.00 0.00	3A4 3A4
MOTA	3490	CG	LEU	481	23.971	1.830	16.194 17.135	1.00	0.00	3A4
ATOM	3491	CD1		481 481	25.057 22.767	1.273 0.861	16.168	1.00	0.00	3A4
ATOM ATOM	3492 3493	CD2 C	LEU	481	23.664	4.637	14.398	1.00	0.00	3A4
ATOM	3494	<u>o</u> .	LEU	481	24.121	5.774	14.349	1.00	0.00	3A4
ATOM	3495	N	LEU	482	23.838	3.733	13.398	1.00	0.00	3A4
ATOM	3496	CA	LEU	482	24.486	3.984	12.124	1.00	0.00	3A4
ATOM	3497	СВ	LEU	482	25.613	2.951	11.765	1.00	0.00	3A4 3A4
MOTA	3498	CG	LEU	482	26.965 27.722	3.067 4.365	12.517 12.213	1.00	0.00	3A4
ATOM	3499 3500	CD1		482 482	26.897	2.808	14.028	1.00	0.00	3A4
ATOM ATOM	3501	C	LEU	482	23.378	3.835	11.115	1.00	0.00	3A4
ATOM	3502	ō	LEU	482	22.784	2.766	11.044	1.00	0.00	3A4
ATOM	3503	N	GLN	483	23.090	4.887	10.291	1.00	0.00	3A4
MOTA	3504	CA	GLN	483	22.131	4.849	9.194	1.00	0.00	3A4 3A4
ATOM	3505	СВ	GLN	483	21.199	6.105	9.194	1.00	0.00	3A4 3A4
ATOM	3506	CG	GLN	483	20.316 19.134	6.274 5.295	10.449 10.458	1.00	0.00	3A4
MOTA	3507 3508	CD	GLN GLN	483 483	18.982	4.423	9.605	1.00	0.00	3A4
ATOM ATOM	3509	NE2		483	18.236	5.459	11.467	1.00	0.00	3A4
ATOM	3510	c	GLN	483	22.916	4.815	7.900	1.00	0.00	3A4
ATOM	3511	0	GLN	483	23.541	5.820	7.606	1.00	0.00	3A4
ATOM	3512	N	PRO	484	22.951	3.748	7.093	1.00	0.00	3A4 3A4
MOTA	3513	CA	PRO	484	23.817	3.721	5.925 7.687	1.00	0.00	3A4
ATOM	3514	CD	PRO	484 484	22.874 24.769	2.409 2.558	6.262	1.00	0.00	3A4
ATOM ATOM	3515 3516	CB CG	PRO PRO	484	23.861	1.520	6.915	1.00	0.00	3A4
ATOM	3517	c	PRO	484	23.035	3.412	4.673	1.00	0.00	3A4
ATOM	3518	ō	PRO	484	21.816	3.307	4.680	1.00	0.00	3A4
ATOM	3519	N	GLU	485	23.773	3.212	3.562	1.00	0.00	3A4
ATOM	3520	ÇA	GLU	485	23.248	2.558	2.383	1.00	0.00	3A4 3A4
ATOM	3521	CB	GLU	485	23.098	3.493 4.316	1.177 0.781	1.00	0.00	3A4
ATOM	3522 3523	CG CD	GTN GTN	485 485	24.327 24.829	3.771	-0.540	1.00	0.00	3A4
ATOM ATOM	3523		GLU	485	24.837	4.541	-1.536	1.00	0.00	3A4
ATOM	3525		GLU	485	25.209	2.571	-0.567	1.00	0.00	3A4
ATOM	3526	С	GLU	485	24.043	1.288	2.206	1.00	0.00	3A4
ATOM	3527	0	GLU	485	25.260	1.289	2.296	1.00	0.00	3A4 3A4
MOTA	3528	N	LYS	486	23.368	0.126	2.027 1.973	1.00	0.00	3A4
ATOM	3529	CA	LYS	486 486	24.038 23.286	-1.172 -2.272	2.791	1.00	0.00	3A4
ATOM ATOM	3530 3531	CB CG	LYS LYS	486	24.070	-3.558	3.141	1.00	0.00	. 3A4
MOTA	3532	CD	LYS	486	24.136	-4.672	2.074	1.00	0.00	3A4
ATOM	3533	CE	LYS	486	22.782	-5.249	1.626	1.00	0.00	3A4
ATOM	3534	NZ	LYS	486	22.037	-5.839	.2.765	1.00	0.00	3A4.
MOTA	3535	C,	LYS	486	24.427	-1.507	0.545	1.00	0.00	3A4 3A4
ATOM	3536	0	LYS	486	25.595 23.564	-1.841 -1.396	0.334 -0.475	1.00	0.00	. 3A4
ATOM ATOM	3537 3538	N CA	PRO PRO	487 487	23.980	-1.646	-1.846	1.00	0.00	3A4
MOTA	3539	CD	PRO	487	22.127	-1.666	-0.334	1.00	0.00	3A4
MOTA	3540	СВ	PRO	487	22.967	-2.687	-2.354	1.00	0.00	3A4
MOTA	3541	CG	PRO	487	21.658	-2.329	-1.638	1.00	0.00	3A4
MOTA	3542	С	PRO	487	23.927	-0.353	-2.647	1.00	0.00	3A4 3A4
MOTA	3543	0	PRO	487	22.999 24.915	0.443	-2.510 -3.541	1.00	0.00	3A4
ATOM	3544	N CA	VAL	488 488	24.946	1.001	-4.417	1.00	0.00	3A4
ATOM ATOM	3545 3546	CB	VAL	488	25.614	2.234	-3.794	1.00	0.00	3A4
ATOM	3547		VAL	488	26.927	1.920	-3.030	1.00	0.00	3A4
ATOM	3548		VAL	488	25.731	3.431	-4.776	1.00	0.00	3A4
ATOM	3549	C	VAL	488	25.663	0.556	-5.657	1.00	0.00	3A4 3A4
MOTA	3550	0	VAL	488	26.886	0.485	-5.692 -6.743	1.00	0.00	3A4 3A4
ATOM	3551	N	VAL	489	24.905 25.452	0.264 -0.202	-8.007	1.00	0.00	3A4
MOTA MOTA	3552 3553	CA CB	VAL VAL	489 489	24.587	-1.266	-8.687	1.00	0.00	3A4
ATOM	3554		VAL	489	25.369	-1.938	-9.848		0.00	3A4
ATOM	3555		VAL	489	24.212	-2.339	-7.638		0.00	3A4
ATOM	3556	c	VAL	489	25.702	0.999	-8.916		0.00	3A4
ATOM	3557	0	VAL	489	24.854	1.864	-9.093	1.00	0.00	3A4

ATOM	3558	N	LEU	490	26.915	1.064	-9.499	1.00	0.00	3A4
MOTA	3559	CA	LEU	490	27.387		-10.386	1.00	0.00	3A4
ATOM	3560	CB	LEU	490	28.695 29.556	2.765	-9.828 -10.717	1.00	0.00	3A4 3A4
ATOM ATOM	3561 3562	CG CD1	LEU	490 490	30.364	4.675	-9.816	1.00	0.00	3A4
ATOM	3563	CD2		490	30.579		-11.694	1.00	0.00	3A4
ATOM	3564	С	LEU	490	27.689		-11.710	1.00	0.00	3A4
ATOM	3565	0	LEU	490	28.311		-11.714	1.00	0.00	3A4 3A4
ATOM	3566	N	LYS	491 491	27.223 27.177		-12.824 -14.188	1.00	0.00	3A4
ATOM ATOM	3567 3568	CA CB	LYS	491	25.982	•	-14.965	1.00	0.00	3A4
ATOM	3569	CG	LYS	491	25.687	1.704	-16.388	1.00	0.00	3A4
ATOM	3570	CD	LYS	491	25.319		-16.460	1.00	0.00	3A4 3A4
ATOM	3571	CE	LYS	491 491	25.043 24.678			1.00	0.00	3A4
ATOM ATOM	3572 3573	NZ C	LYS	491	28.494		-14.912	1.00	0.00	3A4
ATOM	3574	ŏ	LYS	491	29.380	0.964	-14.854	1.00	0.00	3A4
ATOM	3575	N	VAL	492	28.641		-15.620	1.00	0.00	3A4
MOTA	3576	CA	VAL	492	29.700		-16.574 -17.838	1.00	0.00	3A4 3A4
ATOM ATOM	3577 3578	CB CG1	VAL VAL	492 492	29.112 28.415		-17.550 -17.560	1.00	0.00	3A4
ATOM	3579		VAL	492	30.130		-19.001	1.00	0.00	3A4
ATOM	3580	С	VAL	492	30.777		-15.898	1.00	0.00	3A4
MOTA	3581	0	VAL	492	30.519		-14.911	1.00	0.00	3A4 3A4
ATOM	3582	N CA	GLU	493 493	32.030 33.215		-16.415 -15.836	1.00	0.00	3A4
ATOM ATOM	3583 3584	CB	GLU	493	33.962		-14.901	1.00	0.00	3A4
ATOM	3585	CG	GLU	493	34.397		-15.502	1.00	0.00	3A4
MOTA	3586	CD	GLU	493	35.792		-16.141	1.00	0.00	3A4
ATOM	3587		GLU	493	36.769		-15.402 -17.372	1.00	0.00	3A4 3A4
ATOM ATOM	3588 3589	OE2 C	GLU	493 493	35.901 34.100		-16.967	1.00	0.00	3A4
ATOM	3590	ŏ	GLU	493	33.928		-18.117	1.00	0.00	3A4
ATOM	3591	N	SER	494	35.109		-16.624	1.00	0.00	3A4
ATOM	3592	CA	SER	494	36.209		-17.480	1.00	0.00	3A4 3A4
ATOM	3593	CB	SER	494 494	36.076 35.765		-18.010 -16.990	1.00	0.00	3A4
ATOM ATOM	3594 3595	OG C	SER	494	37.455		-16.647	1.00	0.00	3A4
ATOM	3596	ŏ	SER	494	37.360		-15.452	1.00	0.00	3A4
ATOM	3597	N	ARG	495	38.664		-17.262	1.00	0.00	3A4 3A4
ATOM	3598	CA	ARG	495 495	39.886 40.090		-16.587 -16.590	1.00	0.00	3A4
ATOM ATOM	3599 3600	CB CG	ARG	495	39.845		-17.916	1.00	0.00	3A4
ATOM	3601	CD	ARG	495	39.764		-17.697	1.00	0.00	3A4
MOTA	3602	NE	ARG	495	39.301		-18.966	1.00	0.00	3A4
ATOM	3603	CZ	ARG	495	38.710		-18.992 -20.185	1.00	0.00	3A4 3A4
ATOM ATOM	3604 3605	-	ARG ARG	495 495	38.289		-17.853	1.00	0.00	3A4
ATOM	3606		ARG	495	41.073		-17.202	1.00	0.00	. 3A4
ATOM	3607	0	ARG		41.144		-18.413	1.00	0.00	3A4
ATOM	3608	N	ASP	496	42.044		-16.320 -16.647	1.00	0.00	3A4 3A4
ATOM ATOM	3609 3610	CA CB	ASP ASP	496 496	43.290 43.159		-16.860	1.00	0.00	3A4
ATOM	3611	CG		496	42.410		-15.743	1.00		3A4
ATOM	3612		ASP	496	43.070	10.614	-15.056	1.00	0.00	3A4
ATOM	3613		ASP	496	41.179		-15.577	1.00	0.00	3A4 3A4
ATOM	3614 3615	С 0	ASP ASP	496 496	44.272 44.432		-15.553 -15.283	1.00	0.00	3A4
ATOM ATOM	3616	N	GLY	497	44.958		-14.898	1.00	0.00	3A4
ATOM	3617	CA	GLY	497	45.950	7.790	-13.872	1.00	0.00	3A4
ATOM	3618	С	GLY	497	46.12		-13.031	1.00	0.00	3A4 3A4
MOTA	3619	0	GLY	497 498	46.263 46.12		-13.557 -11.677	1.00	0.00	3A4
ATOM ATOM	3620 3621	N CA	THR THR	_	46.35		-10.674	1.00	0.00	3A4
ATOM	3622	CB	THR		45.07		-9.995	1.00	0.00	3A4
MOTA	3623	OG1	THR		44.19		-9.600	1.00	0.00	3A4
ATOM	3624		THR		44.33 47.29		-10.957 -9.640	1.00	0.00	3A4 3A4
ATOM ATOM	3625 3626	0	THR THR		47.29		-9.326	1.00		3A4
ATOM	3627	N	VAL		48.20		-9.074	1.00	0.00	3A4
ATOM	3628	ÇA	VAL	499	49.12	9.727	-8.014	1.00		3A4
ATOM	3629	CB	VAL	499	50.27	2 8.816	-8.476	1.00	0.00	3A4

ATOM	3630	CG1	VAL	499 .	51.133	9.436	-9.607	1.00	0.00	3A4
ATOM	3631		VAL	499	51.110	8.313	-7.273	1.00	0.00	3A4
MOTA	3632	С	VAL	499	49.614	11.021	-7.391	1.00	0.00	3A4
ATOM	3633	0	VAL	499	49.977	11.961	-8.097	1.00	0.00	3A4
ATOM	3634	N	SER	500	49.647	11.075	-6.030	1.00	0.00	3A4
ATOM	3635	CA	SER	500	50.251	12.152	-5.269	1.00	0.00	3A4
MOTA	3636	СВ	SER	500	49.434	13.486	-5.230	1.00	0.00	3A4
ATOM	3637	OG	SER	500	48.086	13.306	-4.816	1.00	0.00	3A4
ATOM	3638	С	SER	500	50.524	11.618	-3.882	1.00	0.00	3A4
ATOM	3639	0	SER	500	49.694	10.933	-3.286	1.00	0.00	3A4
ATOM	3640	N	GLY	501	51.736	11.945	-3.355	1.00	0.00	3A4
ATOM	3641	CA	GLY	501	52.249	11.543	-2.061	1.00	0.00	3A4
ATOM	3642	C	GLY	501	53.489	10.727	-2.291	1.00	0.00	3A4
ATOM	3643	0	GLY	501	54.576	11.087	-1.841	1.00	0.00	3A4
ATOM	3644	N	ALA	502	53.331	9.596	-3.020	1.00	0.00	3A4
MOTA	3645	CA	ALA	502	54.406	8.722	-3.424	1.00	0.00	3A4
ATOM	3646	СВ	ALA	502	54.772	7.642	-2.379	1.00	0.00	3A4
MOTA	3647	Ċ	ALA	502	53.912	8.031	-4.704	1.00	0.00	3A4
MOTA	3648		ALA	502	54.439	8.364	-5.800	1.00	0.00	3A4
ATOM	3649		ALA	502	52.987	7.178	-4.607	1.00	0.00	3A4
TER	3650		ALA	502						
HETATM		FE	HEM	600	33.118	10.391	15.288	1.00	0.00	HEM
HETATM		NA	HEM	600	31.497	11.115	16.171	1.00	0.00	HEM
HETATM		NB	HEM	600	32.274	10.658	13.514	1.00	0.00	HEM
HETATM		NC	HEM	600	34.752	9.684	14.430	1.00	0.00	HEM
HETATM		ND	HEM	600	33.949	10.106	17.065	1.00	0.00	HEM
HETATM			HEM	600	31.254	11.251	17.515	1.00	0.00	HEM
НЕТЛТМ		C2A		600	29.887	11.659	17.752	1.00	0.00	HEM
HETATM			HEM	600	29.316	11.871	16.542	1.00	0.00	HEM
НЕТАТМ			HEM	600	30.322	11.523	15.568	1.00	0.00	HEM
HETATM			HEM	600	31.012	11.136	13.233	1.00	0.00	HEM
HETATM			HEM	600	30.761	11.218	11.804	1.00	0.00	HEM
HETATM			HEM	600	31.901	10.761	11.185	1.00	0.00	HEM
HETATM			HEM	600	32.828	10.426	12.273	1.00	0.00	HEM
HETATM			HEM	600	35.044	9.645	13.089	1.00	0.00	HEM
HETATM			HEM	600	36.395	9.168	12.838	1.00	0.00	HEM
HETATM			HEM	600	36.920	8.833	14.067	1.00	0.00	HEM
HETATM			HEM	600	35.879	9.167	15.033	1.00	0.00	HEM
HETATM			HEM	600	35.150	9.494	17.358	1.00	0.00	HEM
HETATM			HEM	600	35.382	9.408	18.787	1.00	0.00	HEM
HETATM			HEM	600	34.329	10.035	19.375	1.00	0.00	HEM
HETATM			HEM	600	33.438	10.439	18.306	1.00	0.00	HEM
HETATM			HEM	600	32.186	10.978	18.500	1.00	0.00	HEM
HETATM			HEM	600	30.115	11.530	14.204	1.00	0.00	HEM
HETATM	3674	CHC	HEM	600	34.131	9.963	12.102	1.00	0.00	HEM
HETATM	3675	CHD	HEM	600	36.032	9.062	16.407	1.00	0.00	HEM
HETATM	3676	CMA	HEM	600	27.911	12.344	16.281	1.00	0.00	HEM
HETATM	3677	CAA	HEM	600	29.208	11.695	19.088	1.00	0.00	HEM
HETATM	3678	CBA	HEM	600	29,154	13.045	19.638	1.00	0.00	HEM
HETATM	3679	CGA	HEM	600	28.459	13.237	20.946	1.00	0.00	HEM
HETATM	3680	Ola	HEM	600	28.097	12.278	21.566	1.00	0.00	HEM
HETATM	3681	O2A	HEM	600	28.217	14.323	21.438	1.00	0.00	HEM
HETATM	3682	CMB	HEM	600	29.483	11.742	11.185	1.00	0.00	HEM
HETATM	3683	CAB	HEM	600	32.219	10.602	9.818	1.00	0.00	HEM
HETATM	3684	СВВ	HEM	600	31.527	10.978	8.735	1.00	0.00	HEM
HETATM			HEM	600	37.047	9.116	11.471	1.00	0.00	HEM
HETATM	3686		HEM	600	38.159	8.288	14.465	1.00	0.00	HEM
HETATM	3687		HEM	600	39.265	8.069	13.758	1.00	0.00	HEM
HETATM			HEM	600	36.499	8.680	19.483	1.00	0.00	HEM
HETATM		CAD		600	34.101	10.253	20.849	1.00	0.00	HEM
HETATM		CBD		600	34.689	11.583	21.366	1.00	0.00	HEM
HETATM		CGD		600	34.355	11.863	22.843	1.00	0.00	HEM
HETATM			HEM	600	35.050	12.735	23.424	1.00	0.00	HEM
HETATM		02D		600	33.381	11.284	23.380	1.00	0.00	HEM
END									•	

Table	4								*****		101					
Table 4		oviain (P3A7	g the	COOL	aina	ices	01 1	ne c	.IP3A	moc	161					-
TITLE		DEL O	F HUMA	W C	TOCE	ROME	E P45	50 CY	(P3A7	1						
AUTHOR	N.	LOIS														
SEQRES		459							LEU							
SEQRES	_	459							CYS CYS							
SEQRES SEQRES		459 459							ILE							
SEQRES		459							THR							
SEQRES	_	459	PRO	VAL	GLY	PHE	MET	LYS	ASN	ALA	ILE	SER	ILE	ALA	GLU	
SEQRES	7	459	ASP	GLU	GLU	TRP	LYS	ARG	ILE	ARG	SER	LEU	LEU	SER	PRO	
SEQRES		459	THR	PHE	THR	SER	GLY	LYS	LEU	LYS	GLU	MET	VAL	PRO	ILE	
SEQRES		459	ILE	ALA	GLN	TYR	GLY	ASP	VAL LYS	PEO	VAL.	THE	LEU	LYS	HIS	
SEQRES SEQRES		459 459		GTO	GI.Y	A.I.A	TYR	SER	MET	ASP	VAL	ILE	THR	SER	THR	
SEQRES		459							ASP							
SEQRES		459	ASP	PRO	PHE	VAL	GLU	ASN	THR	LYS	LYS	LEU	LEU	ARG	PHE	
SEQRES	14	459							VAL							
SEQRES		459							LEU							
SEQRES		459							ILE							
SEQRES SEQRES		459 459							LEU							
SEQRES		459	GLN	ASN	SER	LYS	ASP	SER	GLU	THR	HIS	LYS	ALA	LEU	SER	
SEQRES		459	ASP	LEU	GLU	LEU	MET	ALA	GLN	SER	ILE	ILE	PHE	ILE	PHE	
SEQRES		459	ALA	GLY	TYR	GLU	THR	THR	SER	SER	VAL	LEU	SER	PHE	ILE	
SEQRES		459	ILE	TYR	GLU	LEU	ALA	THR	HIS	PRO	ASP	VAL	GLN	GLN	LYS	
SEQRES		459 459							THR VAL							
SEQRES SEQRES		459							THR							
SEQRES		459							VAL							
SEQRES	27	459							PRO							
SEQRES		459	ILE	PRO	SER	TYR	VAL	LEU	HIS	HIS	ASP	PRO	LYS	TYR	TRP	
SEQRES		459	THR	GLU	PRO	GLU	LYS	PHE	LEU ASP	PRO	GLU	ARG	TYP	THE	PRO	
SEQRES SEQRES	_	459 459							ASN							
SEQRES		459							LEU							
SEQRES		459	GLN	ASN	PHE	SER	PHE	LYS	PRO	CYS	LYS	GLU	THR	GLN	ILE	
SEQRES		459	PRO	LEU	LYS	LEU	ARG	PHE	GLY	GLY	LEU	LEU	LEU	THR	GLU	
SEQRES		459						LYS	ALA	GLU	SER	ARG	ASP	GLU	THR	
SEQRES HET	36 H EM	459 600		SER	GLI	ALA										
HETNAM		HEM							*							
HETSYN	HEM	3,7	,12,1	7-TE	rami	ETHY:	L-8,	13-D	IVIN	YL-2	,18-	PORP	HINE	DIPR	OPIONIC	ACID
FORMUL	HEM	C34	H34 t		FE:		·	_		_						227
MOTA	1		PRO	45			.768		.244		.895			0.00 0.00		3A7 3A7
ATOM ATOM	2		PRO PRO	45 45			.053 .705		.448		.648 .064			0.00		3A7
ATOM	4		PRO	45			. 467		.950		. 422			0.00		3A7
ATOM	5		PRO -				. 292		.018		.139	1.	00	0.00		3A7
ATOM	6		PRO	45			. 594		.801		.950			0.00		3A7
ATOM	7		PRO	45			.387		.010		.057			0.00		3A7 3A7
ATOM ATOM	8 9		PHE PHE	46 46			.870 .751		.857 .140		.600 .472			0.00		3A7
ATOM	10		PHE	46			.853		.416					0.00		3A7
ATOM	11		PHE	46			.083		.887	-11	. 553	1.		0.00	•	3A7
MOTA	12	CD1		46			.173		.033					0.00		3A7
MOTA	13	CD2		46			.155		.189					0.00		3A7 3A7
MOTA MOTA	14 15	CE1		46 46			.317 .297		.474					0.00		3A7
ATOM	16	CE2	PHE	46			.380		.775				00	0.00		3A7
ATOM	17		PHE	46			.491		.691		.782			0.00		3A7
MOTA	18	0	PHE	46		19	. 400	5	.166		.096		00	0.00		3A7
ATOM	19		LEU	47			. 629		.749		.814		00	0.00		3A7
ATOM	20		LEU	47			.541		.204		.035 .874		00 00	0.00		3A7 3A7
ATOM ATOM	21 22		LEU LEU	47 47			.661 .490		.667 .978		.129		00	0.00		3A7
ATOM	23	CD1		47			.133		.202		.826		00	0.00		3A7
ATOM	24	CD2		47			.768	-0	.526	-5	.942	1.	00	0.00		3A7
MOTA	25		LEU	47			.573		.860		.681		00	0.00		3A7
ATOM	26		LEU	47			.619		. 930		.036		00	0.00		3A7 3A7
ATOM ATOM	27 28		GLY GLY	48 48			.396		.349		.225 .933		00 00	0.00		3A7
UIT	20	~~		7.0		10	0	- 4		-						

ATOM	29	С	GLY	48	16.930	4.491	-3.395	1.00	0.00	3A7
ATOM	30	0	GLY	48	15.938	5.218	-3.414	1.00	0.00	3A7 3A7
ATOM	31 32	N CA	ASN ASN	49 49	16.911 15.741	3.229 2.585	-2.898 -2.348	1.00	0.00	3A7
ATOM ATOM	33	CB	ASN	49	15.445	1.235	-3.059	1.00	0.00	3A7
ATOM	34	CG	ASN	49	14.046	0.705	-2.706	1.00	0.00	3A7
ATOM	35	OD1	ASN	49	13.035	1.349	-3.011	1.00	0.00	3A7
ATOM	36		ASN	49	14.005	-0.494	-2.051	1.00	0.00	3A7 3A7
ATOM	37	C	ASN	49	16.016 17.169	2.375 2.278	-0.880 -0.463	1.00	0.00	3A7
ATOM ATOM	38 39	N	ASN ALA	49 50	14.933	2.293	-0.065	1.00	0.00	3A7
ATOM	40	CA	ALΛ	50	14.998	2.111	1.369	1.00	0.00	3A7
ATOM	41	CB	ALA	50	13.847	2.834	2.098	1.00	0.00	3A7
MOTA	42	С	ALA	50	14.941	0.641	1.697	1.00	0.00	3A7 3A7
ATOM	43	0	λLA	50 51	13.866 16.133	0.049 0.032	1.787 1.885	1.00	0.00	3A7
ATOM ATOM	44 45	N CA	LEU	51	16.271	-1.360	2.232	1.00	0.00	3A7
ATOM	46	CB	LEU	51	16.271	-2.314	1.001	1.00	0.00	3A7
ATOM	47	CG	LEU	51	17.055	-1.862	~0.262	1.00	0.00	3A7
MOTA	48		LEU	51	18.587	-1.811	-0.098	1.00	0.00	3A7 3A7
ATOM	49		LEU	· 51	16.690 17.550	-2.765 -1.468	-1.456 3.012	1.00	0.00	3A7
ATOM ATOM	50 51	С 0	LEU	51 51	18.327	-0.517	3.085	1.00	0.00	3A7
ATOM	52	N	SER	52	17.794	-2.657	3.613	1.00	0.00	3A7
ATOM	53	CA	SER	52	19.005	-2.956	4.343	1.00	0.00	3A7
ATOM	54	CB	SER	52	18.741	-3.361	5.821	1.00	0.00	3A7 3A7
ATOM	55 56	OG	SER	52	17.737 19.734	-4.363 -4.023	5.945 3.562	1.00	0.00	3A7
ATOM ATOM	56 57	С 0	SER	52 52	20.164	-3.782	2.435	1.00	0.00	3A7
ATOM	58	N	PHE	53	19.898	-5.231	4.155	1.00	0.00	3A7
. ATOM	59	CA	PHE	53	20.599	-6.341	3.550	1.00	0.00	3A7
MOTA	60	СВ	PHE	53	21.908	-6.703	4.297	1.00	0.00	3A7 3A7
ATOM :	61 62	CG	PHE	53 53	22.730 22.819	-5.456 -4.809	4.439 5.673	1.00	0.00	3A7
ATOM ATOM	63		PHE	53	23.346	-4.880	3.327	1.00	0.00	3A7
ATOM	. 64		PHE	53	23.491	3.598	5.793	1.00	0.00	3A7
ATOM	65	CE2	PHE	53	24.018	-3.667	3.446	1.00	0.00	3A7
MOTA	66	CZ	PHE	53	24.085	-3.022	4.675	1.00	0.00	3A7 3A7
ATOM ATOM	67 68	С 0	PHE	53 53	19.639 19.885	-7.494 -8.495	3.594 4.264	1.00	0.00	3A7
ATOM	69	N	ARG	54	18.491	-7.330	2.875	1.00	0.00	3A7
ATOM	70	CA	ARG	54	17.327	-8.205	2.828	1.00	0.00	3A7
MOTA	71	СВ	ARG	54	17.629	-9.719	2.641	1.00	0.00	3A7
ATOM	72	CG	ARG	54	18.536 17.996	-10.045 -9.573	1.437 0.079	1.00	0.00	3A7 3A7
ATOM ATOM	73 74	CD NE	ARG	54 54	19.049	-9.836	-0.962	1.00	0.00	3A7
ATOM	75	CZ	ARG	54	19.036	-10.925	-1:791	1.00	່0.00	3A7
ATOM	76	NH1	ARG	54	20.065	-11.113	-2.669	1.00	0.00	3A7
MOTA	77		ARG	54	18.013	-11.826	-1.753	1.00	0.00	3A7 3A7
MOTA	78 79	С О	ARG ARG	54 54	16.514 16.760	-7.983 -8.611	4.087 5.116	1.00	0.00	3A7
ATOM ATOM	80	N	LYS	55	15.545	-7.030	4.028	1.00	0.00	3A7
ATOM	81	CA	LYS	55	14.927	-6.447	5.205	1.00	0.00	3A7
ATOM	82	CB	LYS	55	14.520	-4.971	5.023	1.00	0.00	3A7
ATOM	83	CG	LYS	55 55	13.327 13.574	-4.656	4.092 2.582	1.00	0.00	3A7 3A7
ATOM ATOM	84 85	CD	LYS	55 55	13.574	-4.842 -6.171	1.993	1.00	0.00	3A7
ATOM	86	NZ	LYS	55	11.612	-6.322	2.178	1.00	0.00	3A7
ATOM	87	С	LYS	55	13.767	-7.241	5.777	1.00	0.00	3A7
ATOM	88	0	LYS	55	13.403	-7.067	6.938	1.00	0.00	3A7 3A7
ATOM	89	N	GLY	56 56	13.158 12.066	-8.146 -8.950	4.991 5.491	1.00	0.00	3A7 3A7
ATOM ATOM	90 91	CA C	GLY GLY	56 56		-10.146	4.604	1.00	0.00	3A7
ATOM	92	ŏ	GLY	56		-10.334	3.823	1.00	0.00	3A7
ATOM	93	N	TYR	57	13.009	-11.031	4.730	1.00	0.00	3A7
ATOM	94	CA	TYR	57		-12.222	3.922	1.00	0.00	3A7 3A7
ATOM	95 96	CB CG	TYR TYR	57 57		-12.913 -13.558	4.319 3.146	1.00	0.00	3A7
MOTA MOTA	96 97		TYR	57		-12.832	1.995	1.00	0.00	3A7
ATOM	98		TYR	57	15.566	-14.898	3.223	1.00	0.00	3A7
MOTA	99	CE1	TYR	57		-13.440	0.934	1.00	0.00	3A7
MOTA	100	CE2	TYR	57	16.240	-15.506	2.168	1.00	0.00	3A7

ATOM	101	CZ	TYR	57	16.538	-14.777	1.021	1.00	0.00	3A7
ATOM	102	OH	TYR	57	17.229	-15.392	-0.043	1.00	0.00	3A7
MOTA	103	С	TYR	57	12.013	-13.191	4.022	1.00	0.00	3A7
ATOM	104	0	TYR	57		-13.781	3.021	1.00	0.00	3A7
ATOM	105	N	TRP	58		-13.353	5.211	1.00	0.00	3A7
MOTA	106	CA	TRP	58		-14.269	5.359	1.00	0.00	3A7
ATOM	107	СВ	TRP	58		-14.515	6.832	1.00	0.00	3A7 3A7
ATOM	108	CG	TRP	58		-13.318	7.606	1.00	0.00	3A7 3A7
ATOM	109		TRP	58		-13.247	8.157	1.00	0.00	3A7
ATOM	110		TRP	58 58		-12.115 -11.297	7.871 8.548	1.00	0.00	3A7
ATOM ATOM	111 112		TRP	58		-11.978	8.741	1.00	0.00	3A7
ATOM	112		TRP	58		-14.158	8.175	1.00	0.00	3A7
ATOM	114		TRP	58		-11.604	9.360	1.00	0.00	3A7
ATOM	115		TRP	58		-13.780	8.796	1.00	0.00	3A7
ATOM	116		TRP	58		-12.522	9.382	1.00	0.00	3A7
ATOM	117	С	TRP	58	9.036	-13.824	4.612	1.00	0.00	3A7
ATOM	118	0	TRP	58	8.302	-14.664	4.106	1.00	0.00	3A7
ATOM	119	N	THR	59	8.780	-12.490	4.502	1.00	0.00	3A7
ATOM	120	CA	THR	59	7.645	-11.989	3.737	1.00	0.00	3A7
ATOM	121	CB	THR	59		-10.582	4.136	1.00	0.00	3A7
ATOM	122	OG1	THR	59	8.282	-9.643	4.073	1.00	0.00	3A7
ATOM	123	CG2	THR	59		-10.634	5.579	1.00	0.00	3A7
ATOM	124	C	THR	59		-12.067	2.267	1.00	0.00	3A7
ATOM	125	0	THR	59		-12.232	1.471	1.00	0.00	3A7
MOTA	126	N	PHE	60		-12.018	1.884	1.00	0.00	3A7
ATOM	127	CA	PHE	60		-12.244	0.530	1.00	0.00	3A7
ATOM	128	CB	PHE	60		-11.803	0.330	1.00	0.00	3A7
ATOM	129	CG	PHE	60		-11.735	-1.126	1.00	0.00	3A7 3A7
ATOM	130		PHE	60		-10.822	-1.978	1.00	0.00	3A7
ATOM	131		PHE	60		-12.595	-1.647		0.00	3A7
ATOM	132		PHE	60		-10.772 -12.548	-3.328 -2.997	1.00	0.00	3A7
ATOM	133 134	CEZ	PHE	60 60		-11.636	-3.839	1.00	0.00	3A7
ATOM	135	C C	PHE	60		-13.695	0.122	1.00	0.00	3A7
MOTA MOTA	136	ō	PHE	60		-14.011	-0.936	1.00	0.00	3A7
ATOM	137	N	ASP	61		-14.632	0.991	1.00	0.00	3A7
ATOM	138	CA	ASP	61		-16.051	0.737	1.00	0.00	3A7
ATOM	139	СВ	ASP	61		-16.892	1.774	1.00	0.00	3A7
ATOM	140	CG	ASP	61		-16.729	1.612	1.00	0.00	3A7
ATOM	141		ASP	61	12.612	-16.736	0.447	1.00	0.00	3A7
ATOM	142	OD2	ASP	61	12.818	-16.555	2.655	1.00	0.00	3A7
ATOM	143	С	ASP	61,	8.415	-16.503	0.698	1.00	0.00	- 3A7
ATOM	. 144	0	ASP	61	8.070	-17.371	-0.085	1.00	0.00	3A7
ATOM	145	N	MET	62		-15.870	1.491	1.00	0.00	3A7
ATOM	146	CA	MET	62		-16.134	1.452	1.00	0.00	3A7
ATOM	147	СВ	MET	62		-15.468		1.00	0.00	3A7
ATOM	148	CG	MET	62		-16.224	3,947	1.00	0.00	· 3A7
MOTA	149	, SD	MET	62		-15.359	5.422	1.00	0.00	
ATOM	150	CE	MET	62		-15.481	5.031	1.00	0.00	3A7 3A7
ATOM	151	Ç	MET	62		-15.672	0.168	1.00	0.00	3A7
ATOM	152	0	MET	62 63		-16.335 -14.555	-0.342 -0.430	1.00	0.00	3A7
ATOM	153 154	N	GLU	63			-1.722	1.00	0.00	3A7
MOTA MOTA	155	CA CB	GLU GLU	63		-12.683	-2.039	1.00	0.00	3A7
ATOM	156	CG	GLU	63		-11.593	-1.206	1.00	0.00	3A7
ATOM	157	CD	GLU	63		-10.239	-1.427	1.00	0.00	3A7
ATOM	158		GLU	63		-10.169	-2.214	1.00	0.00	3A7
ATOM	159		GLU	63	5.495	-9.249	-0.802	1.00	0.00	3A7
ATOM	160	С	GLU	63		-15.044	-2.831	1.00	0.00	3A7
ATOM	161	o	GLU	63	5.087	-15.339	-3.734	1.00	0.00	3A7
ATOM	162	N	CYS	64	7.093	-15.606	-2.747	1.00	0.00	3A7
ATOM	163	CA	CYS	64	7.601	-16.598	-3.674	1.00	0.00	3A7
ATOM	164	CB	CYS	64		-16.969	-3.362	1.00	0.00	3A7
MOTA	165	SG	CYS	64		-15.524	-3.736	1.00	0.00	3A7
MOTA	166	С	CYS	64		-17.853	-3.631	1.00	0.00	3A7
MOTA	167	0	CYS	64		-18.402	-4.655	1.00	0.00	3A7
ATOM	168	N	TYR	65		-18.323	-2.413	1.00	0.00	3A7
ATOM	169	CA	TYR	65		-19.526	-2.251	1.00	0.00	3A7
ATOM	170	CB	TYR	65		-19.993	-0.802	1.00	0.00	3A7
ATOM	171	CG	TYR	65		-20.246	-0.379	1.00	0.00	3A7
ATOM	172	CD1	TYR	65	7,458	-19.725	0.834	1.00	0.00	3A7

ATOM	173	CD2	TYR	65	7.985	-20.850	-1.222	1.00	0.00	3A7
ATOM	174	CEl	TYR	65	8.800	-19.750	1.182	1.00	0.00	3A7
ATOM	175	CE2	TYR	65		-20.816	-0.901	1.00	0.00	3A7
ATOM	176	CZ	TYR	65		-20.216	0.283	1.00	0.00	3A7
ATOM	177	ОН	TYR	65		-20.003	0.572	1.00	0.00	3A7
ATOM	178	C	TYR	65		-19.373	-2.701	1.00	0.00	3A7 3A7
ATOM	179	0	TYR	65 66		-20.319 -18.174	-3.228 -2.556	1.00	0.00	3A7
ATOM ATOM	180 181	N CA	LYS LYS	66		-17.922	-3.043	1.00	0.00	3A7
ATOM	182	CB	LYS	66		-16.564	-2.544	1.00	0.00	3A7
ATOM	183	CG	LYS	66		-16.579	-1.049	1.00	0.00	3A7
ATOM	184	CD	LYS	66		-15.185	-0.470	1.00	0.00	3A7
ATOM	185	CE	LYS	66	-0.063	-14.502	-1.089	1.00	0.00	3A7
ATOM	186	NZ	LYS	66		-13.182	-0.461	1.00	0.00	3A7
ATOM	187	С	LYS	66		-17.957	-4.556	1.00	0.00	3A7
ATOM	188	0	LYS	66		-18.326	-5.129	1.00	0.00	3A7
MOTA	189	N	LYS	67		-17.595	-5.243	1.00	0.00	3A7
MOTA	190	CA	LYS	67 67		-17.539	-6.682 -7.137	1.00	0.00	3A7 3A7
MOTA MOTA	191 192	CB CG	LYS LYS	67 67		-16.414 -16.145	-8.651	1.00	0.00	3A7
ATOM	193	CD	LYS	67 ·		-14.878	-9.034	1.00	0.00	3A7
ATOM	194	CE	LYS	67		-14.629		1.00	0.00	3A7
ATOM	195	NZ	LYS	67		-14.424		1.00	0.00	3A7
ATOM	196	С	LYS	67	3.853	-18.855	-7.284	1.00	0.00	3A7
ATOM	197	0	LYS	67	3.254	-19.336	-8.244	1.00	0.00	3A7
ATOM	198	N	TYR	68		-19.451	-6.748	1.00	0.00	3A7
ATOM	199	CA	TYR	68		-20.573	-7.355	1.00	0.00	3A7
ATOM	200	СВ	TYR	68		-20.402	-7.314	1.00	0.00	3A7
ATOM	201	CG	TYR	68		-19.259 -17.989	-8.216 -7.702	1.00 1.00	0.00	3A7 3A7
ATOM ATOM	202 203		TYR TYR	68 68		-19.457	-9.595	1.00	0.00	3A7
ATOM	204		TYR	68		-16.937	-8.550	1.00	0.00	3A7
ATOM	205		TYR	68		-18.408		1.00	0.00	3A7
ATOM	206	CZ	TYR	68		-17.146	-9.924	1.00	0.00	3A7
ATOM	207	OH	TYR	68	8.537	-16.080	-10.784	1.00	0.00	3A7
ATOM	208	С	TYR	68		-21.899	-6.770	1.00	0.00	· 3A7
ATOM	209	0	TYR	68		-22.918	-7.453	1.00	0.00	3A7
ATOM	210	N	ARG	69		-21.912	-5.500	1.00	0.00	3A7 3A7
ATOM	211	CA CB	ARG	69 69		-23.040 -23.733	-4.856 -5.717	1.00	0.00	3A7 3A7
ATOM ATOM	212 213	CG	ARG ARG	69		-22.762	-6.180	1.00	0.00	3A7
ATOM	214	CD	ARG	69		-23.441	-7.009	1.00	0.00	3A7
ATOM	215	NE	ARG	69		-23.933	-8.287	1.00	0.00	3A7
ATOM	216	CZ	ARG	69		-24.664	-9.197	1.00	0.00	3A7
ATOM	217	NH1	ARG	69	1.345	-25.083	-10.347	1.00	0.00	3A7
ATOM	218	NH2		69		-24.981	-8.963	1.00	0.00	3A7
ATOM	219	С	ARG	69		-23.968	-4.257	1.00	0.00	3A7
ATOM	220	0	ARG	₋ 69		-23.556	-3.663	1.00	0.00	3A7 3A7
ATOM .	221 222	N CA	LYS LYS	70 70		-25.251 -26.459	-4.585 -4.410	1.00 1.00	0.00	3A7
ATOM	223	CB	LYS	70 70		-27.726	-4.955	1.00	0.00	3A7
ATOM	224	CG	LYS	70		-28.142		1.00	0.00	3A7
ATOM	225	CD	LYS	70		-27.345	-4.536	1.00	0.00	3A7
ATOM	226	CE	LYS	70	1.635	-27.577	-5.929	1.00	0.00	3A7
MOTA	227	NZ	LYS	70		-26.976	-7.009	1.00	0.00	3A7
ATOM	228	С	LYS	70		-26.352	-5.122	1.00	0.00	3A7
MOTA	229	0	LYS	70		-26.860	-6.233	1.00	0.00	3A7°
ATOM	230	N	VAL	71		-25.662	-4.449	1.00	0.00	3A7 3A7
MOTA MOTA	231 232	CA CB	VAL	71 71		-25.641 -26.967	-4.770 -5.362	1.00	0.00	3A7 3A7
ATOM	233	CG1	VAL VAL	71		-26.882	-5.635	1.00	0.00	3A7
ATOM	234	CG2	VAL	71		-28.158	-4.411	1.00	0.00	3A7
ATOM	235	C	VAL	71		-24.472	-5.708	1.00	0.00	3A7
ATOM	236	ō	VAL	71		-24.376	-6.751	1.00	0.00	3A7
MOTA	237	N	TRP	72		-23.545	-5.337	1.00	0.00	3A7
MOTA	238	CA	TRP	72		-22.433	-6.182	1.00	0.00	3A7
MOTA	239	CB	TRP	72		-21.089	-5.839	1.00	0.00	3A7
MOTA	240	CG	TRP	72		-19.873	-5.306	1.00	0.00	3A7
MOTA MOTA	241	CD2		72 72		-18.737 -19.633	-6.108 -4.054	1.00	0.00	3A7 3A7
ATOM	242 243	CD1 NE1		72 72		-19.633	-4.034	1.00	0.00	3A7
ATOM	244	CE2		72		-17.866	-5.277	1.00	0.00	3A7

ATOM	245	CE3	TRP	72	10.923	-18.434	-7.436	1.00	0.00	3A7
ATOM	246		TRP	72	12.368	-16.672	-5.760	1.00	0.00	3A7
ATOM	247		TRP	72	11.414	-17.223	-7.920	1.00	0.00	3A7
ATOM	248		TRP	72	12.124	-16.354	-7.094	1.00	0.00	3A7
ATOM	249	C	TRP	72	12.229	-22.293	-6.064	1.00	0.00	3A7
ATOM	250	o	TRP	72	12.824	-22.782	-5.112	1.00	0.00	3A7
ATOM	251	N	GLY	73	12.861	-21.582	-7.022	1.00	0.00	3A7
ATOM	252	CA	GLY	73	14.278	-21.323	-6.985	1.00	0.00	3A7
ATOM	253	С	GLY	73		-19.850	-6.821	1.00	0.00	3A7
ATOM	254	o	GLY	73	13.812	-19.031	-7.409	1.00	0.00	3A7
ATOM	255	N	ILE	74		-19.484	-6.009	1.00	0.00	3A7
ATOM	256	CA	ILE	74		~18.120	-5.754	1.00	0.00	3A7
ATOM	257	CB	ILE	74		-17.676	-4.328	1.00	0.00	3A7
ATOM	258		ILE	74		-18.543	-3.258	1.00	0.00	3A7
ATOM	259	CG1	ILE	74	15.835	-16.159	-4.124	1.00	0.00	3A7
ATOM	260	CD	ILE	74		-15.621	-2.836	1.00	0.00	3A7
ATOM	261	C	ILE	74		-18.077	-6.023	1.00	0.00	3A7
ATOM	262	ō	ILE	74	18.100	-19.082	-5.904	1.00	0.00	3A7
ATOM	263	N	TYR	75		-16.900	-6.425	1.00	0.00	3A7
ATOM	264	CA	TYR	75		-16.765	-6.827	1.00	0.00	3A7
ATOM	265	СВ	TYR	75		-16.348	-8.308	1.00	0.00	3A7
ATOM	266	CG	TYR	75		-17.400	-9.184	1.00	0.00	3A7
ATOM	267		TYR	75		-17.281	-9.613	1.00	0.00	3A7
ATOM	268		TYR	75		-18.513	-9.582	1.00	0.00	3A7
ATOM	269		TYR	75		-18.261		1.00	0.00	3A7
ATOM	270		TYR	75		-19.489		1.00	0.00	3A7
ATOM	271	CZ	TYR	75		-19.367		1.00	0.00	3A7
ATOM	272	ОН	TYR	75		-20.361		1.00	0.00	3A7
ATOM	273	c	TYR	75		-15.716	-5.954	1.00	0.00	3A7
ATOM	274	ŏ	TYR	75		-14.543	-6.059	1.00	0.00	3A7
ATOM	275	N	ASP	76		-16.106	-5.059	1.00	0.00	3A7
ATOM	276	CA	ASP	76		-15.171	-4.194	1.00	0.00	3A7
ATOM	277	СВ	ASP	76		-15.513	-2.685	1.00	0.00	3A7
ATOM	278	CG	ASP	76		-15.259	-2.172	1.00	0.00	3A7
ATOM	279		ASP	76		-15.935	-2.652	1.00	0.00	3A7
ATOM	280		ASP	76		-14.382	-1.279	1.00	0.00	3A7
ATOM	281	c	ASP	76		-15.175	-4.597	1.00	0.00	3A7
ATOM	282	ŏ	ASP	76		-16.000	-4.149	1.00	0.00	3A7
ATOM	283	N	CYS	77		-14.210	-5.459	1.00	0.00	3A7
ATOM	284	CA	CYS	77		-13.896	-5.902	1.00	0.00	3A7
ATOM	285	СВ	CYS	77		-13.074	-4.858	1.00	0.00	3A7
ATOM	286	SG	CYS	7 7		-13.854	-3.237	1.00	0.00	3A7
ATOM	287	С	CYS	7 7	25.544	-15.056	-6.442	1.00	0.00	3A7
ATOM	288	0	CYS	77	26.561	-15.442	-5.879	1.00	0.00	3A7
ATOM	289	N	GLN	78	25.091	-15.613	-7.583	1.00	0.00	3A7
ATOM	290	CA	GLN	78	25.770	-16.622	-8.369	1.00	0.00	3A7
ATOM	291	CB	GLN	78	27.325	-16.549	-8.440	1.00	0.00	3A7
ATOM	292	CG	GLN	78	27.848	-15.222	-9.017	1.00	0.00	3A7
ATOM	293	CD	GLN	78 .	29.378	-15.274	-9.063	1.00	0.00	3A7
ATOM	294	OE1	GLN	78	29.961	-16.057	-9.823	1.00	0.00	3A7
ATOM	295	NE2	GLN	78	30.031	-14.415	-8.222	1.00	0.00	3A7
ATOM	296	С	GLN	78	25.375	-18.037	-8.023	1.00	0.00	`3A7
ATOM	297	0	GLN	78	25.715	-18.949	-8.771	1.00	0.00	3A7
ATOM	298	N	GLN	79	24.653	-18.277	-6.903	1.00	0.00	3A7
ATOM	299	CA	GLN	.79	24.270	-19.620	-6.516	1.00	0.00	3A7
ATOM	300	CB	GLN	79	24.718	-19.978	-5.085	1.00	0.00	3A7
ATOM	301	CG	GLN	79	26.242	-19.895	-4.897	1.00	0.00	3A7
ATOM	302	CD	GLN	79	26.582	-20.276	-3.453	1.00	0.00	3A7
ATOM	303	OEl	GLN	79	26.176	-19.589	-2.508	1.00	0.00	3A7
ATOM	304	NE2	GLN	79	27.346	-21.399	-3.294	1.00	0.00	3A7
MOTA	305	С	GLN	79	22.765	-19.774	-6.615	1.00	0.00	3A7
MOTA	306	0	GLN	79		-18.847	-6.260	1.00	0.00	3A7
ATOM	307	N	PRO	80		-20.926		1.00	0.00	3A7
ATOM	308	CA	PRO	80		-21.225		1.00	0.00	3A7
MOTA	309	CD	PRO	80		-21.867		1.00	0.00	3A7
MOTA	310	CB	PRO	80		-22.191		1.00	0.00	3A7
MOTA	311	CG	PRO	80		-22.915		1.00	0.00	3A7
ATOM	312	С	PRO	80		-21.899		1.00	0.00	3A7
MOTA	313	0	PRO	80		-22.746		1.00	0.00	3A7
ATOM	314	N	MET	81		-21.571		1.00	0.00	3A7
MOTA	315	CA	MET	81		-22.233		1.00	0.00	3A7
MOTA	316	CB	MET	81	19.098	-21.392	-2.669	1.00	0.00	3A7

ATOM	317	CG	MET	81	20.582	-21.043	-2.428	1.00	0.00	3A7
ATOM	318	SD	MET	81	20.947	-20.209	-0.854	1.00	0.00	3A7
MOTA	319	CE	MET	81	20.120		-1.276	1.00	0.00	3A7
ATOM	320	С	MET	81	17.447		-4.177	1.00	0.00	3A7
ATOM	321	0	MET	81	16.677		-4.447	1.00	0.00	3A7 3A7
ATOM	322	N	LEU	82		-23.763	-4.052	1.00	0.00	3A7
ATOM	323	CA	LEU	82		-24.130	-4.201 -4.990	1.00	0.00	3A7
ATOM	324	CB	LEU	82		-25.434 -25.122	-6.509	1.00	0.00	3A7
ATOM	325	CG	LEU	82 82		-25.569	-7.137	1.00	0.00	3A7
ATOM ATOM	326 327		TEA .	82		-25.622	-7.300	1.00	0.00	3A7
ATOM	328	C	LEU	82		-24.179	-2.843	1.00	0.00	3A7
ATOM	329	ŏ	LEU	82		-24.903	-1.947	1.00	0.00	3A7
MOTA	330	N	ALA	83	13.975	-23.351	-2.673	1.00	0.00	3A7
ATOM	331	CA	ALA	83		-23.210	-1.443	1.00	0.00	3A7
MOTA	332	CB	ALA	83		-21.792	-1.267	1.00	0.00	3A7
ATOM	333	C	ALA	83		-24.096	-1.430	1.00	0.00	3A7 3A7
MOTA	334	0	ALA	83		-24.025	-2.320 -0.399	1.00	0.00	3A7
ATOM	335	М	ILE	84		-24.967 -25.985	-0.290	1.00	0.00	3A7
ATOM	336 337	CA CB	ILE	84 84		-27.364	0.009	1.00	0.00	3A7
ATOM ATOM	338		ILE	84		-28.307	0.374	1.00	0.00	3A7
ATOM	339		ILE	84		-28.016	-1.243	1.00	0.00	3A7
ATOM	340	CD	ILE	84		-27.201	-2.013	1.00	0.00	3A7
ATOM	341	C	ILE	84		-25.576	0.802	1.00	0.00	3A7
ATOM	342	0	ILE	84		-25.289	1.921	1.00	0.00	3A7
ATOM	343	N	THR	85		-25.597	0.509	1.00	0.00	3A7
MOTA	344	CA	THR	85		-25.139	1.413	1.00	0.00	3A7 3A7
ATOM	345	CB	THR	85		-23.819	0.999	1.00	0.00	3A7
ATOM	346		THR	85		-23.627 -22.782	-0.412 1.725	1.00	0.00	3A7
ATOM	347 348	C C	THR THR	85 85		-26.125	1.486	1.00	0.00	3A7
ATOM ATOM	349	Ö	THR	85		-26.730	0.619	1.00	0.00	3A7
ATOM	350	N	ASP	86		-26.396	2.502	1.00	0.00	3A7
ATOM	351	CA	ASP	86		-27.263	2.510	1.00	0.00	3A7
ATOM .	352	CB	ASP	86	3.722	-27.421	1.361	1.00	0.00	3A7
ATOM	353	CG	ASP	86		-26.055	0.952	1.00	0.00	3A7
ATOM	354		ASP	86		-25.362	1.833	1.00	0.00	· 3A7
MOTA	355		ASP	86		-25.692	-0.246	1.00	0.00	3A7 3A7
ATOM	356	C	ASP	86		-28.602 -28.994	3.011 2.738	1.00	0.00	3A7
MOTA	357	O N	ASP PRO	86 87		-29.324	3.756	1.00	0.00	3A7
ATOM ATOM	358 359	CA	PRO	87		-30.519	4.472	1.00	0.00	3A7
ATOM	360	CD	PRO	87		-28.734	4.388	1.00	0.00	3A7
ATOM	361	СВ	PRO	87	3.599	-30.942	5.276	1.00	0.00	3A7
MOTA	362	CG	PRO	87	2.505	-29.914	4.977	1.00	0.00	3A7
MOTA	363	С	PRO	87		-31.641	3.571	1.00	0.00	3A7
MOTA	364	0	PRO	87		-32.375	3.920	1.00	0.00	3A7 3A7
MOTA	365	N	ASP.	88	•	-31.800	2.413	1.00	0.00	3A7
ATOM	366	CA	ASP	88		-32.846 -32.701	1.455 0.270	1.00	0.00	3A7
MOTA MOTA	367 368	CB ⁻ CG	ASP ASP	88 88		-32.826	0.749	1.00	0.00	3A7
ATOM	369		ASP	88		-33.640	1.676	1.00	0.00	3A7
ATOM	370		ASP	88		-32.094	0.198	1.00	0.00	3A7
ATOM	371	С	ASP	88		-32.787	0.909	1.00	0.00	3A7
ATOM	372	0	ASP	88		-33.798	0.830	1.00	0.00	3A7
MOTA	373	N	MET	. 89		-31.588	0.554	1.00	0.00	3A7
MOTA	374	CA	MET	89		-31.388	0.009	1.00	0.00	3A7 3A7
ATOM	375	СВ	MET	89		-30.073	-0.773 -1.918	1.00	0.00	3A7
MOTA	376	CG	MET	89		-30.035 -28.663	-1.731	1.00	0.00	3A7
MOTA	377 378	SD	MET MET	89 89		-27.425	-1.755	1.00	0.00	3A7
MOTA MOTA	379	C	MET	89		-31.390	1.081	1.00	0.00	3A7
ATOM	380	ŏ	MET	89		-31.936	0.893	1.00	0.00	3A7
ATOM	381	N	ILE	90		-30.824	2.267	1.00	0.00	3A7
ATOM	382	CA	ILE	90		-30.812	3.398	1.00	0.00	3A7
MOTA	383	CB	ILE	90		-29.908	4.501	1.00	0.00	3A7
MOTA	384		ILE	90		-30.036	5.807	1.00	0.00	3A7
MOTA	385		ILE	90		-28.467	3.973	1.00	0.00	3A7 3A7
ATOM	386	CD	ILE	90		-27.853	3.815 3.920	1.00		3A7
ATOM	387	C	ILE	90		-32.218 -32.588	4.248	1.00		3A7
MOTA	388	0	ILE	90	11.010	-32,300	7.240	1.00	5.00	

ATOM	389	N	LYS	91	8.877	-33.100	3.925	1.00	0.00	3A7
ATOM	390	CA	LYS	91		-34.479	4.328	1.00	0.00	3A7
ATOM	391 _	СВ	LYS	91		-35.240	4.361	1.00	0.00	3A7
ATOM	392	CG	LYS	91		-36.619	5.036	1.00	0.00	3A7
ATOM	393	CD	LYS	91		-37.269	5.192	1.00	0.00	3A7 3A7
ATOM	394	CE	LYS	91		-38.628 -39.206	5.898 6.031	1.00	0.00	3A7
MOTA	395	NZ	LYS LYS	91 91		-35.200	3.414	1.00	0.00	3A7
MOTA MOTA	396 397	C O	LYS	91		-36.021	3.838	1.00	0.00	3A7
ATOM	398	N	THR	92		-34.861	2.113	1.00	0.00	3A7
ATOM	399	CA	THR	92		-35.382	1.113	1.00	0.00	3A7
MOTA	400	СВ	THR	92		-34.980	-0.272	1.00	0.00	3A7
MOTA	401		THR	92	9.047	-35.206	-0.430	1.00	0.00	3A7
ATOM	402	CG2	THR	92	11.180	-35.836	-1.323	1.00	0.00	3A7
ATOM	403	С	THR	92		-34.904	1.326	1.00	0.00	3A7
MOTA	404	0	THR	92		-35.657	1.196	1.00	0.00	3A7
ATOM	405	N	VAL	93		-33.620	1.730	1.00	0.00	3A7
MOTA	406	CA	VAL	93		-33.006	1.938	1.00	0.00	3A7 3A7
ATOM	407	CB	VAL	93 93		-31.500 -30.752	2.127 1.061	1.00	0.00	3A7
ATOM	408 409		VAL VAL	93		-31.074	3.585	1.00	0.00	3A7
MOTA MOTA	410	C	VAL	93		-33.705	3.034	1.00	0.00	3A7
ATOM	411	ŏ	VAL	93		-33.627	3.002	1.00	0.00	3A7
ATOM	412	N	LEU	94		-34.522	3.946	1.00	0.00	3A7
MOTA	413	CA	LEU	94		-35.450	4.889	1.00	0.00	3A7
ATOM	414	СВ	LEU	94	13.538	-36.540	5.429	1.00	0.00	3A7
ATOM	415	CG	LEU	94	12.454	-36.028	6.397	1.00	0.00	3A7
ATOM	416	CD1	LEU	94		-37.136	6.726	1.00	0.00	3A7
ATOM	417	CD2	LEU	94		-35.489	7.687	1.00	0.00	3A7
ATOM	418	C	LEU	94		-36.253	4.325	1.00	0.00	3A7
ATOM	419	0	LEU	94		-36.171	4.842	1.00	0.00	3A7
ATOM	420	N	VAL	95 05		-37.041	3.249	1.00	0.00	3A7 3A7
ATOM	421	CA	VAL	95 05		-37.904 -37.147	2.446 1.449	1.00	0.00	3A7
ATOM ATOM	422 423	CB	VAL VAL	95 95		-36.331	2.088	1.00	0.00	3A7
ATOM	424		VAL	95		-38.131	0.379	1.00	0.00	3A7
ATON	425	c	VAL	95		-38.932	3.269	1.00	0.00	3A7
ATOM	426	ō	VAL	95		-38.606	4.052	1.00	0.00	3A7
ATOM	427	N	LYS	96	16.651	-40.226	3.099	1.00	0.00	3A7
ATOM	428	CA	LYS	96	17.216	-41.310	3.864	1.00	0.00	3A7
ATOM	429	СВ	LYS	96		-41.757	5.021	1.00	0.00	3A7
ATOM	430	CG	LYS	96		-42.863	5.922	1.00	0.00	3A7
ATOM	431		LYS	96		-43.296	7.055	1.00	0.00	3A7
ATOM	432	CE	LYS	96		-42.211	8.105 8.783	1.00	0.00	3A7 3A7
ATOM	433 434	NZ C	LYS LYS	96 96		-41.808 -42.463	2.917	1.00	0.00	3A7
ATOM ATOM	435	0	LYS	96		-42.998	2.397	1.00	0.00	3A7
ATOM	436	N	GLU	97		-42.930	2.649	1.00	0.00	3A7
ATOM	437	CA	GLU	97		-42.451	3.016	1.00	0.00	3A7
ATOM	438	CB	GLU	97		-41.024	2.498	1.00	0.00	3A7
ATOM	439	CG	GLU	97	20.271	-40.894	0.966	1.00	0.00	3A7
ATOM	440	CD	GLU	97		-41.763	0.314	1.00	0.00	3A7
ATOM	441		GLU	97		-42.695	-0.447	1.00	0.00	3A7
ATOM	442		GLU	97		-41.504	0.567	1.00	0.00	3A7
ATOM	443	С	GLU	97		-42.531	4.499	1.00	0.00	3A7
ATOM	444	0	GLU	97		-41.560	5.238	1.00	0.00	3A7 3A7
ATOM	445	N	CYS	98		-43.711 -43.956	4.956 6.327	1.00	0.00	3A7
ATOM ATOM	446 447	CA CB	CYS CYS	98 98		-45.456	6.703	1.00	0.00	3A7
ATOM	448	SG	CYS	98		-46.111	6.530	1.00	0.00	3A7
ATOM	449	c	CYS	98		-43.454	6.538	1.00	0.00	3A7
ATOM	450	ŏ	CYS	98		-43.131	7.656	1.00	0.00	3A7
ATOM	451	N	TYR	99		-43.358	5.423	1.00	0.00	3A7
ATON	452	CA	TYR	99		-42.699	5.352	1.00	0.00	3A7
ATOM	453	CB	TYR	99		-43.602	4.775	1.00	0.00	3A7
ATOM	454	CG	TYR	99		-44.708	5.749	1.00	0.00	3A7
ATOM	455		TYR	99		-45.981	5.553	1.00	0.00	3A7
MOTA	456		TYR	99		-44.471	6.875	1.00	0.00	3A7
ATOM	457		TYR	99		-47.000	6.470	1.00	0.00	3A7 3A7
ATOM	458		TYR	99 99		-45.488 -46.754	7.791 7.591	1.00	0.00	3A7
ATOM ATOM	459 460	C2 OH	TYR TYR	99 99		-47.785	8.524	1.00	0.00	3A7
A I ON	100	On	1114	23	20.007	103	0.344	1.00	0.00	5.11

ATOM	461	С	TYR	99	24.459	-41.520	4.445	1.00	0.00	3A7
ATOM	462	0	TYR	99	24.717	-41.584	3.244	1.00	0.00	3A7
MOTA	463	N	SER	100	23.943		5.029	1.00	0.00	3A7
MOTA	464	CA	SER	100	23.548		4.317	1.00	0.00	3A7 3A7
ATOM	465	CB	SER	100	22.340 22.547		4.990 6.381	1.00	0.00	3A7
ATOM	466 467	og C	SER SER	100 100	24.721		4.207	1.00	0.00	3A7
ATOM ATOM	468	o	SER	100	25.295		5.211	1.00	0.00	3A7
ATOM	469	N	VAL	101	25.093		2.947	1.00	0.00	3A7
ATOM	470	CA	VAL	101		-37.096	2.616	1.00	0.00	3A7
ATOM	471	СВ	VAL	101	26.925		1.327	1.00	0.00	3A7
ATOM	472	CG1		101		-36.746	1.143	1.00	0.00 0.00	3A7 3A7
ATOM	473	CG2	VAL	101	27.188	-39.049 -35.663	1.394 2.512	1.00	0.00	3A7
ATOM ATOM	474 475	C	VAL VAL	101 101		-35.187	1.447	1.00	0.00	3A7
ATOM	476	N	PHE	102		-34.944	3.658	1.00	0.00	3A7
ATOM	477	CA	PHE	102		-33.531	3.774	1.00	0.00	3A7
ATOM	478	СВ	PHE	102	24.757	-33.208	5.051	1.00	0.00	3A7
ATOM	479	CG	PHE	102		-31.734	5.284	1.00	0.00	3A7
ATOM	480	CD1		102	24.224		4.236	1.00	0.00	3A7 3A7
ATOM	481	CD2		102		-31.227 -29.493	6.582 4.481	1.00	0.00	3A7
ATOM	482 483	CE1		102 102		-29.870	6.830	1.00	0.00	3A7
ATOM ATOM	484	CZ	PHE	102		-29.000	5.777	1.00	0.00	3A7
ATOM	485	C	PHE	102		-32.887	3.838	1.00	0.00	3A7
ATOM	486	Ó	PHE	102	27.728	-33.174	4.741	1.00	0.00	3A7
ATOM	487	N	THR	103		-31.980	2.869	1.00	0.00	3A7
ATOM	488	CA	THR	103		-31.281	2.757 1.308	1.00	0.00	3A7 3A7
MOTA	489	CB	THR THR	103 103		-30.904 -30.496	1.135	1.00	0.00	3A7
ATOM ATOM	490 491		THR	103		-29.816	0.779	1.00	0.00	3A7
ATOM	492	c	THR	103		-30.083	3.685	1.00	0.00	3A7
ATOM	493	o	THR	103		-29.672	4.169	1.00	0.00	3A7
ATOM	494	N	ASN	104		-29.507	3.955	1.00	0.00	3A7
ATOM	495	CA	ASN	104		-28.430	4.899	1.00	0.00	3A7 3A7
ATOM	496	CB	ASN	104		-28.320 -28.168	5.343 4.161	1.00	0.00	3A7
ATOM ATOM	497 498	CG OD1	ASN ASN	104 104		-27.047	3.775	1.00	0.00	3A7
ATOM	499		ASN	104		-29.333	3.597	1.00	0.00	3A7
ATOM	500	С	ASN	104	29.418	-27.105	4.342	1.00	0.00	3A7
ATOM	501	.0	ASN.	104		-26.868	3.135	1.00	0.00	3A7
ATOM	502	N	ARG	105		-26.205	5.250	1.00	0.00	3A7 3A7
ATOM	503	CA	ARG	105		-24.859 -24.275	4.929 5.967	1.00	0.00	3A7
ATOM ATOM	504 505	CB CG	ARG ARG	105 105		-25.018	6.037	1.00	0.00	3A7
ATOM		CD	ARG	105		-24.418	7.111	1.00	0.00	 3A7
ATOM	507	NE	ARG	105		-25.205	7.173	1.00	0.00	3A7
ATOM	508	CZ .	ARG	105		-24.845	8.007	1.00	0.00	3A7
ATOM .	509		ARG	105		-25.583	8.027	1.00	0.00	3A7
ATOM	510		ARG	105		-23.752 -23.977	8.816 4.884	1.00	0.00	3A7 3A7
ATOM	511	c o	ARG ARG	105 105		-24.170	5.645	1.00	0.00	3A7
ATOM ATOM	512 513	N	ARG	106		-22.991	3.955	1.00	0.00	3A7
ATOM	514	CA	ARG	106		-22.177	3.639		0.00	3A7
ATOM	515	СВ	ARG	106		-21.586	2.205	1.00	0.00	3A7
ATOM	516	CG	ARG	106		-22.664	1.121	1.00	0.00	3A7
MOTA	517	CD	ARG	106		-22.088	-0.292	1.00	0.00	3A7 3A7
ATOM	518	NE	ARG	106	-	-21.318 -20.619	-0.652 -1.824	1.00	0.00	3A7
ATOM ATOM	519 520	CZ	ARG ARG	106 106		-19.927	-2.100	1.00	0.00	3A7
ATOM	521		ARG	106		-20.607	-2.718	1.00	0.00	3A7
ATOM	522	С	ARG	106		-21.087	4.647	1.00	0.00	3A7
ATOM	523	0	ARG	106 ·		-20.971	5.015	1.00	0.00	3A7
ATOM	524	N	PRO	107		-20.287	5.178	1.00	0.00	 3A7
ATOM	525	CA	PRO	107		-19.212	6.105	1.00	0.00	3A7 • 3A7
ATOM	526 527	CD	PRO	107 107		-20.159 -18.456	4.663 6.287	1.00	0.00	3A7
ATOM ATOM	527 528	CB CG	PRO	107		-18.724	4.991	1.00	0.00	3A7
ATOM	529	C	PRO	107		-19.732	7.435	1.00	0.00	3A7
ATOM	530	ŏ	PRO	107		-19.045	8.098	1.00	0.00	3A7
ATOM	531	N	PHE	108		-20.949	7.846	1.00	0.00	3A7
MOTA	532	CA	PHE	108	30.989	-21.534	9.116	1.00	0.00	3A7

ATOM	533	СВ	PHE	108	29.984	-22.623	9.543	1.00	0.00	3A7
ATOM	534	CG	PHE	108	28.575	-22.099	9.639	1.00	0.00	3A7
MOTA	535		PHE	108		-21.852	8.488	1.00	0.00	3A7 3A7
ATOM ATOM	536 537		PHE	108 108		-21.924 -21.446	10.885 8.575	1.00	0.00	3A7 3A7
ATOM	538		PHE	108		-21.528	10.976	1.00	0.00	3A7
ATOM	539	CZ	PHE	108		-21.298	9.821	1.00	0.00	3A7
MOTA	540	С	PHE	108		-22.153	9.070	1.00	0.00	3A7
MOTA	541	0	PHE	108		-22.269	10.095	1.00	0.00	3A7
MOTA	542	N	GLY	109		-22.555 -23.135	7.875 7.691	1.00	0.00	3A7 3A7
ATOM ATOM	543 544	CA C	GLY	109 109		-23.133	8.056	1.00	0.00	3A7
ATOM	545	ŏ	GLY	109		-22.774	8.561	1.00	0.00	3A7
ATOM	546	N	PRO	110		-20.938	7.853	1.00	0.00	3A7
ATOM	547	CA	PRO	110		-20.023	8.270	1.00	0.00	3A7
ATOM	548	CD	PRO	110		-20.430	6.620	1.00	0.00	3A7 3A7
ATOM ATOM	549 550	CB CG	PRO PRO	110 110		-18.682 -19.054	7.743 6.361	1.00	0.00	3A7
ATOM	551	c	PRO	110		-19.895	9.765	1.00	0.00	3A7
ATOM	552	ō	PRO	110		-19.525	10.094	1.00	0.00	3A7
ATOM	553	N	VAL	111		-20.153	10.690	1.00	0.00	3A7
ATOM	554	CA	VAL	111		-19.847	12.107	1.00	0.00	3A7
ATOM ATOM	555 556	CB	VAL VAL	111 111		-19.678 -18.645	12.890 12.147	1.00	0.00	3A7 3A7
ATOM	557		VAL	111		-21.007	13.118	1.00	0.00	3A7
ATOM	558	c	VAL	111		-20.855	12.787	1.00	0.00	3A7
ATOM	559	0	VAL	111		-22.067	12.658	1.00	0.00	3A7
ATOM	560	N	GLY	112		-20.325	13.502	1.00	0.00	3A7
ATOM	561	CA	GLY	112 112		-21.102 -20.384	14.130 13.863	1.00	0.00	· 3A7
ATOM ATOM	562 563	С 0	GLY	112		-19.155	13.891	1.00	0.00	3A7
ATOM	564	N	PHE	113		-21.162	13.582	1.00	0.00	3A7
ATOM	565	CA	PHE	113		-20.640	13.182	1.00	0.00	3A7
ATOM	566	CB	BHE	113		-20.476	14.380	1.00	0.00	3A7
ATOM	567 568	CG	PHE	113 113		-19.854 -20.468	13.980 14.346	1.00	0.00	3A7 3A7
ATOM ATOM	569		PHE	. 113		-18.671	13.239	1.00	0.00	3A7
ATOM	570		PHE	113		-19.918	13.971	1.00	0.00	`3A7
MOTA	571		PHE	113		-18.120	12.861	1.00	0.00	3A7
MOTA	572	CZ	PHE	113		-18.744	13.226	1.00	0.00	3A7
ATOM ATOM	573 574	c o	PHE	113 113		-21.648 -22.372	12.181 12.431	1.00	0.00	3A7 3A7
ATOM	575	N	MET	114		-21.708	11.011	1.00	0.00	3A7
ATOM .	576	CA	MET	114		-22.600	9.882	1.00	0.00	3A7
MOTA	577	CB	MET	114		-22.624	9.331	1.00	0.00	3A7
ATOM	578	ÇG	MET	114		-21.313	8.647	1.00	0.00	3A7
ATOM ATOM	579 580	SD CE	MET MET	114 114		-19.936 -18.779	9.761 8.440	1.00	0.00	3A7 3A7
ATOM	581	C	MET	114		-24.012	10.217	1.00	0.00	3A7
ATOM	582	0	MET	114		-24.294	11.346	1.00	0.00	3A7
ATOM	583	N	LYS	115		-24.924	9.208	1.00	0.00	3A7
ATOM	584	CA	LYS	115		-26.343	9.268	1.00	0.00	3A7 3A7
ATOM ATOM	585 586	CB CG	LYS LYS	115 115		-27.158 -27.432	10.423 10.251	1.00	0.00	3A7
ATOM	587	CD	LYS	115		-26.252	10.533	1.00	0.00	3A7
ATOM	588	CE	LYS	115	44.796	-25.758	11.988	1.00	0.00	3A7
ATOM	589	NZ	LYS	115		-26.832	12.922	1.00	0.00	3A7
ATOM	590	C	LYS	115		-26.569 -26.979	9.300 8.297	1.00	0.00	3A7 3A7
MOTA MOTA	591 592	0 N	LYS ASN	115 116		-26.341	10.491	1.00	0.00	3A7
ATOM	593	CA	ASN	116		-26.560	10.889	1.00	0.00	3A7
ATOM	594	СВ	ASN	116		-25.724	10.133	1.00	0.00	3A7
ATOM	595	CG	ASN	116		-26.079	8.657	1.00	0.00	3A7
ATOM	596	OD1		116		-25.453 -27.074	7.745 8.437	1.00	0.00	3A7 3A7
ATOM ATOM	597 598	ND2 C	ASN	116 116		-28.039	10.949	1.00	0.00	3A7
ATOM	599	ŏ	ASN	116		-28.777	9.979	1.00	0.00	3A7
ATOM	600	N	ALA	117	37.387	-28.501	12.134	1.00	0.00	3A7
ATOM	601	CA	ALA	117		-29.900	12.415	1.00	0.00	3A7
ATOM ATOM	602 603	CB C	ALA ALA	117 117		-30.247 -30.294	13.899 12.024	1.00	0.00	3A7 3A7
ATOM	604	Ö	ALA	117		-30.857	10.951	1.00	0.00	3A7
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ATOM	605	N	ILE	118	34.758	-30.027	12.909	1.00	0.00	3A7
ATOM	606	CA	ILE	118		-30.498	12.732	1.00	0.00	3A7
MOTA	607	СВ	ILE	118		-31.666	13.661	1.00	0.00	3A7
ATOM	608		ILE	118		-32.948	13.008	1.00	0.00	3A7
ATOM	609		ILE	118		-31.523	15.097	1.00	0.00	3A7
ATOM	610	CD	ILE	118		-30.511	15.983	1.00	0.00	3A7
ATOM	611	c	ILE	118		-29.333	12.894	1.00	0.00	3A7
ATOM	612	ŏ	ILE	118		-29.399	13.643	1.00	0.00	3A7
ATOM	613	N	SER	119		-28.231	12.139	1.00	0.00	3A7
ATOM	614	CA	SER	119		-27.054	12.114	1.00	0.00	3A7
ATOM	615	СВ	SER	119		-25.747	11.972	1.00	0.00	3A7
ATOM	616	OG	SER	119		-25.595	13.079	1.00	0.00	3A7
ATOM	617	C	SER	119		-27.178	10.949	1.00	0.00	3A7
ATOM	618	ŏ	SER	119		-26.507	9.930	1.00	0.00	3A7
ATOM	619	N	ILE	120		-28.096	11.093	1.00	0.00	3A7
ATOM	620	CA	ILE	120		-28.576	10.086	1.00	0.00	3A7
ATOM	621	СВ	ILE	120		-27.497	9.294	1.00	0.00	3A7
ATOM	622		ILE	120		-28.166	8.349	1.00	0.00	3A7
ATOM	623		ILE	120		-26.482	10.237	1.00	0.00	3A7
ATOM	624	CD	ILE	120		-27.096	11.166		0.00	3A7
ATOM	625	c	ILE	120		-29.507	9.171	1.00	0.00	3A7
ATOM	626	ō	ILE	120		-29.081	8.276	1.00	0.00	3A7
ATOM	627	N	ALA	121		-30.825	9.421	1.00	0.00	3A7
ATOM	628	CA	ALA	121		-31.779	8.845	1.00	0.00	3A7
ATOM	629	СВ	ALA	121		-32.322	9.891	1.00	0.00	3A7
ATOM	630	c	ALA	121		-32.895	8.190		0.00	3A7
ATOM	631	ō	ALA	121		-33.051	8.369	1.00	0.00	3A7
ATOM	632	N	GLU	122		-33.699	7.384	1.00	0.00	3A7
ATOM	633	CA	GLU	122		-34.785	6.580	1.00	0.00	3A7
ATOM	634	СВ	GLU	122		-34.988	5.292	1.00	0.00	3A7
ATOM	635	CG	GLU	122		-33.676	4.532	1.00	0.00	3A7
ATOM	636	CD	GLU	122		-33.979	3.190	1.00	0.00	3A7
ATOM	637		GLU	122		-34.679	2.360	1.00	0.00	3A7
ATOM	638		GLU	122	32.884	-33.510	2.975	1.00	0.00	3A7
ATOM	639	С	GLU	122	30.077	-36.057	7.368	1.00	0.00	3A7
ATOM	640	0	GLU	122	30.753	-36.091	8.393	1.00	0.00	3A7
ATOM	641	N	ASP	123	29.389	-37.130	6.889	1.00	0.00	3A7
ATOM	642	CA	ASP	123	29.236	-38.402	7.576	1.00	0.00	3A7
ATOM	643	CB	ASP	123	27.977	-39.195	7.107	1.00	0.00	3A7
ATOM	644	CG	ASP	123	28.012	-39.602	5.628	1.00	0.00	3A7
MOTA	645	OD1	ASP	123	28.196	-38.707	4.763	1.00	0.00	3A7
ATOM	646	OD2	ASP	123	27.861	-40.822	5.354	1.00	0.00	3A7
ATOM	647	С	ASP	123	30.485	~39.259	7.471	1.00	0.00	3A7
MOTA	648	0	ASP	123		-39.955	6.485	1.00	0.00	3A7
MOTA	649	N	GLU	124		-39.189	8.540	1.00	0.00	3A7
ATOM	650	CA	GLU	124		-39.870	8.683	1.00	0.00	3A7
ATOM	651	CB	GLU	124		-39.519	7.609	1.00	0.00	3A7
ATOM	652	CG	GLU	124		-40.257	7.793	1.00	0.00	3A7
ATOM	653	CD	GLU.	124		-39.851	6.672	1.00	0.00	3A7
ATOM	654		GLU	124		-39.275	6.989	1.00	0.00	3A7
ATOM	655		GLU	124		-40.115	5.486	1.00	0.00	3A7
ATOM	656	C	GLU	124		-39.381	10.020	1.00	0.00	3A7
ATOM	657	0	GLU	124		-40.149	10.866	1.00	0.00	3A7
ATOM .	658	N	GLU	125		-38.047		1.00	0.00	3A7
ATOM	659	CA	GLU	125		-37.358	11.455	1.00	0.00	3A7
ATOM	660	CB	GLU	125		-36.078	11.267	1.00	0.00	3A7
ATOM	661	CG	GLU	125		-36.303	10.505 11.254	1.00	0.00	3A7 3A7
ATOM	662	CD	GLU	125		-37.314		1.00		3A7
ATOM	663	OE1		125		-38.392 -37.024	10.667	1.00	0.00	3A7
ATOM	664	OE2		125			12.418	1.00		3A7
ATOM	665	C	GLU	125		-36.969	12.096 13.306	1.00	0.00	3A7 3A7
ATOM	666 667	O N	GLU	125 126		-36.775 -36.843	11.315	1.00	0.00	3A7 3A7
ATOM ATOM	668	CA	TRP TRP	126		-36.458	11.855	1.00	0.00	3A7
ATOM	669	CB	TRP	126		-36.001	10.762	1.00	0.00	3A7
ATOM	670	CG	TRP	126		-34.955	11.159	1.00	0.00	3A7
ATOM	671	CD2		126		-33.684	11.776	1.00	0.00	3A7
ATOM	672	CD1		126		-34.933	10.869	1.00	0.00	3A7
ATOM	673	NE1		126		-33.741	11.271	1.00	0.00	3A7
ATOM	674	CE2		126		-32.954	11.818	1.00	0.00	3A7
ATOM	675	CE3		126		-33.139	12.252	1.00	0.00	3A7
ATOM	676	CZ2		126		-31.670	12.329	1.00	0.00	3A7
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ATOM	677	CZ3	TRP	126	28.868	-31.850	12.774	1.00	0.00		3A7
ATOM	678	CH2	TRP	126	27.680	-31.123	12.810	1.00	0.00		3A7
ATOM	679	С	TRP	126		-37.602	12.636	1.00	0.00		3A7
ATOM	680	0	TRP	126		-37.423	13.750	1.00	0.00		3A7
MOTA	681	N	LYS	127		-38.842	12.090	1.00	0.00		3A7
ATOM	682	CA	LYS	127		-40.060	12.743	1.00	0.00		3A7
ATOM	683	СВ	LYS	127		-41.279	11.833	1.00	0.00		3A7 3A7
ATOM	684	CG	LYS	127		-42.581	12.315 11.316	1.00	0.00		3A7
ATOM	685	CD	LYS	127		-43.736 -45.046	11.770	1.00	0.00		3A7
ATOM ATOM	686 687	CE NZ	LYS LYS	127 127		-44.893	11.883	1.00	0.00		3A7
ATOM	688	C	LYS	127		-40.320	14.072	1.00	0.00		3A7
ATOM	689	ŏ	LYS	127		-40.651	15.070	1.00	0.00		3A7
ATOM	690	N	ARG	128		-40.112	14.123	1.00	0.00		3A7
ATOM	691	CA	ARG	128		-40.271	15.331	1.00	0.00		3A7
ATOM	692	СВ	ARG	128	32.812	-40.274	15.061	1.00	0.00		3A7
ATOM	693	CG	ARG	128		~41.515	14.267	1.00	0.00		3A7
ATOM	694	CD	ARG	128		-41.777	14.317	1.00	0.00		3A7
MOTA	695	NE	ARG	128		-41.942	15.749	1.00	0.00		3A7
ATOM	696	CZ	ARG	128		-43.090	16.469	1.00	0.00		3A7
ATOM	697		ARG	128		-43.140	17.776	1.00	0.00		3A7 3A7
ATOM	698		ARG	128		-44.186 -39.217	15.894 16.367	1.00	0.00		3A7
ATOM	699 700	C	ARG	128 128		-39.549	17.535	1.00	0.00	•	3A7
ATOM ATOM	701	O N	ARG ILE	129		-37.931	15.976	1.00	0.00		3A7
ATOM		·CA	ILE	129		-36.852	16.897	1.00	0.00		3A7
ATOM	703	СВ	ILE	129		-35.498	16.229	1.00	0.00		3A7
ATOM	704		ILE	129		-34.398	16.740	1.00	0.00		3A7
ATOM	705		ILE	129		-34.975	16.405	1.00	0.00		3A7
ATOM	706	CD	ILE	129	33.250	-35.944	16.093	1.00	0.00		3A7
ATOM	707	С	ILE	129		-37.028	17.444	1.00	0.00		3A7
MOTA	708	0	ILE	129		-36.896	18.640	1.00	0.00		3A7
ATOM	709	N	ARG	130		-37.398	16.595	1.00	0.00		3A7
MOTA	710	CA	ARG	130		-37.661	17.021	1.00	0.00		3A7
ATOM	711	CB	ARG	130		-37.943	15.811	1.00	0.00		3A7 3A7
	.712	CG	ARG	130 = 1 130		-36.681 -36.942	14.987 13.796	1.00	0.00		3A7
ATOM ATOM	713 714	CD NE	ARG ARG	130		-37.896	12.857	1.00	0.00		3A7
ATOM	715	CZ	ARG	130		-38.311	11.694	1.00	0.00		3A7
ATOM	716		ARG	130		-39.169	10.868	1.00	0.00		3A7
ATOM	717		ARG	130		-37.869	11.351	1.00	0.00	•	3A7
ATOM	718	С	ARG	130	26.695	-38.843	17.970	1.00	0.00		3A7
ATOM	719	0	ARG	130	26.037	-38.756	18.996	1.00	0.00		3A7
MOTA	720	N	SER	131		-39.943	17.701	1.00	0.00		3A7
ATOM	721	CA	SER	131		-41.105	18.571	1.00	0.00		3A7
ATOM	7,22	СВ	SER	131		-42.268	17.985	1.00	0.00		3A7
ATOM ·	723	OG	SER	131		-41.986	17.760	1.00	0.00		3A7 3A7
	724	C	SER	131	•	-40.816	19.936	1.00	0.00		3A7
ATOM	725	.0	SER	131		-41,352 -39.936	20.947 19.998	1.00	0.00	•	3A7
ATOM ATOM	726 727	N CA	LEU	132 132		-39.583	21.240	1.00	0.00		3A7
ATOM	728	СВ	LEU	132		-38.838	20.968	1.00	0.00		3A7
ATOM	729	CG	LEU	132		-39.732	20.333	1.00	0.00		3A7
ATOM	730		LEU	132		-38.875	19.583	1.00	0.00		3A7
ATOM	731		LEU	132	32.782	-40.648	21.366	1.00	0.00		3A7
ATOM	732	С	LEU	132		-38.721	22.089	1.00	0.00		3A7
MOTA	733	0	LEU	132		-38.937	23.289	1.00	0.00		3A7
ATOM	734	N	LEU	133		-37.745	21.460	1.00	0.00		3A7
ATOM	735	CA	LEU	133		-36.794	22.145	1.00	0.00		3A7
ATOM	736	СВ	LEU	133		-35.547	21.272	1.00	0.00		3A7 3A7
ATOM	737	CG	LEU	133		-34.787 -33.493	20.869	1.00	0.00		3A7
ATOM	738 739		LEU	133 133		-33.493	22.052	1.00	0.00		3A7
ATOM ATOM	740	CDZ	LEU	133		-37.334	22.547	1.00	0.00		3A7
ATOM	741	0	TEO	133		-36.955	23.590	1.00	0.00		3A7
ATOM	742	N	SER	134		-38.237	21.738	1.00	0.00		3A7
ATOM	743	CA	SER	134		-38.748	21.970	1.00	0.00		3A7
ATOM	744	СВ	SER	134		-39.662	20.844	1.00	0.00		3A7
MOTA	745	OG	SER	134		-40.706	20.461	1.00	0.00		3A7
MOTA	746	С	SER	134	23,800	-39.430	23.296	1.00	0.00		3A7
MOTA	747	0	SER	134		-39.226	23.854	1.00	0.00		3A7
MOTA	748	N	PRO	135	24.715	-40.198	23.891	1.00	.0.00		3A7

MOTA	749	CA	PRO	135	24.491	-40.773	25.190	1.00	0.00	3A7
MOTA	750	CD	PRO	135	25.854	-40.834	23.260	1.00	0.00	3A7
MOTA	751	CB	PRO	135	25.551	-41.871	25.355	1.00	0.00	
MOTA	752	CG	PRO	135		-42.203	23.924	1.00	0.00	3A7
ATOM	753	С	PRO	135		-39.783	26.310	1.00	0.00	3A7
MOTA	754	0	PRO	135		-39.912	27.273	1.00	0.00	3A7
ATOM	755	N	THR	136		-38.805	26.231	1.00	0.00	3A7 3A7
ATOM	756	CA	THR	136		-37.840	27.291	1.00	0.00	· 3A7
ATOM	757	CB	THR	136		-37.210	27.207 25.918	1.00	0.00	3A7
ATOM	758 759		THR THR	136 136		-36.654 -38.319	27.492	1.00	0.00	3A7
ATOM ATOM	760	C	THR	136		-36.769	27.320	1.00	0.00	3A7
ATOM	761	ŏ	THR	136		-36.212	28.360	1.00	0.00	3A7
ATOM	762	N	PHE	137		-36.471	26.165	1.00	0.00	3A7
ATOM	763	CA	PHE	137	23.044	-35.454	26.069	1.00	0.00	3A7
ATOM	764	СВ	PHE	137	23.219	-34.665	24.778	1.00	0.00	3A7
ATOM	765	CG	PHE	137	24.305	-33.645	25.018	1.00	0.00	3A7
ATOM	766	CD1	PHE	137		-33.792	24.468	1.00	0.00	3A7
ATOM	767		PHE	137		-32.535	25.831	1.00	0.00	3A7
ATOM	768		PHE	137		-32.863	24.725	1.00	0.00	3A7
ATOM	769		PHE	137		-31.590	26.070	1.00	0.00	3A7
ATOM	770	CZ	PHE	137		-31.757	25.524 26.100	1.00	0.00	3A7 3A7
ATOM	771	C	PHE	137		-36.153	25.406	1.00	0.00	3A7
MOTA	772 773	O N	PHE THR	137 138		-35.799 -37.179	26.952	1.00	0.00	3A7
ATOM ATOM	774	CA	THR	138		-37.782	27.179	1.00	0.00	3A7
ATOM	775	CB	THR	138		-39.259	27.505	1.00	0.00	3A7
ATOM	776		THR	138		-39.549	28.518	1.00	0.00	3A7
ATOM	777		THR	138		-40.035	26.226	1.00	0.00	3A7
ATOM	778	С	THR	138	19.588	-37.063	28.326	1.00	0.00	3A7
ATOM	779	0	THR	138		-36.412	29.149	1.00	0.00	3A7
MOTA	780	N	SER	139		-37.211	28.416	1.00	0.00	3A7
ATOM	781	CA	SER	139		-36.585	29.427	1.00	0.00	3A7
ATOM	782	СВ	SER	139		-36.809	29.183	1.00	0.00	3A7
ATOM	783	OG	SER	139		-38.188	29.037	1.00	0.00	3A7 3A7
ATOM	784	C	SER	139 .		-37.053 -36.290	30.810 31.765	1.00	0.00	3A7
ATOM	785 786	O N	SER GLY	139 140		-38.318	30.922	1.00	0.00	3A7
ATOM ATOM	787	CA	GLY	140		-38.898	32.158	1.00	0.00	3A7
ATOM	788	C	GLY	140		-38.362	32.618	1.00	0.00	3A7
ATOM	789	ŏ	GLY	140		-38.260	33.820	1.00	0.00	3A7
ATOM	790	N	LYS	141	20.933	-38.021	31.673	1.00	0.00	3A7
ATOM	791	CA	LYS	141	22.309	-37.803	32.064	1.00	0.00	3A7
ATOM	792	CB	LYS	141		-38.611	31.169	1.00	0.00	3A7
ATOM	793	CG	LYS	141	•	-40.129	31.293	1.00	0.00	3A7
ATOM	794	CD	LYS	141		-40.944	30.571	1.00	0.00	3A7
ATOM	795	CE	LYS	141		-42.456	30.655	1.00	0.00	3A7 3A7
ATOM ATOM	· 796	NZ	LYS	141		-43.189 -36.386	29.928 32.232	1.00	0.00	3A7
ATOM .	797 798	C O	LYS LYS	141 141		-35.680	33.265	1.00	0.00	3A7
ATOM	799	N	LEU	142		-36.031	31.185	1.00	0.00	3A7
ATOM	800	CA	LEU	142		-34.970	31.099	1.00	0.00	3A7
ATOM	801	CB	LEU	142		-33.593	30.894	1.00	0.00	3A7
ATOM	802	CG	LEU	142	24.455	-32.799	29.656	1.00	0.00	3A7
ATOM	803		LEU	142	23.560	-31.564	29.439	1.00	0.00	3A7
ATOM	804	CD2	LEU	142		-32.407	29.718	1.00	0.00	3A7
ATOM	805	С	LEU	142		-34.903	32.241	1.00	0.00	3A7
ATOM	806	0	LEU	142		-33.901	32.398	1.00	0.00	3A7
MOTA	807	N	LYS	143		-35.975	33.085	1.00	0.00	3A7
ATOM	808	CA	LYS	143		-36.077	34.381	1.00	0.00	3A7 3A7
ATOM	809	CB	LYS	143		-35.966 -37.003	34.315 33.373	1.00	0.00	3A7
ATOM ATOM	810 811	CG CD	LYS LYS	143 143		-38.480	33.614	1.00	0.00	3A7
ATOM	812	CE	LYS	143		-39.129	34.873	1.00	0.00	3A7
ATOM	813	NZ	LYS	143		-38.601	36.117	1.00	0.00	3A7
ATOM	814	C	LYS	143		-35.060	35.351	1.00	0.00	3A7
ATOM	815	ŏ	LYS	143		-34.248	35.919	1.00	0.00	3A7
ATOM	816	N	GLU	144		-35.097	35.479	1.00	0.00	3A7
ATOM	817	CA	GLU	144		-34.122	36.090	1.00	0.00	3A7
MOTA	818	СВ	GLU	144		-33.575	37.466	1.00	0.00	3A7
MOTA	819	CG	GLU	144		-34.669	38.535	1.00	0.00	3A7
MOTA	820	CD	GLU.	144	24.730	-34.037	39.820	1.00	0.00	3A7

ATOM	821	OE1	GLU	144	25.849 -34.42	2 40.255	1.00	0.00	3A7
ATOM	822	OE2		144	24.022 -33.16		1.00	0.00	3A7
MOTA	823	С	GLU	144	23.380 -32.97		1.00	0.00	3A7
ATOM	824	0	GLU	144	24.284 -32.16		1.00	0.00 0.00	3A7 3A7
MOTA	825	N	MET	145	22.163 -32.86		1.00 1.00	0.00	3A7
ATOM	826	CA	MET	145	21.768 -31.69 21.203 -31.93		1.00	0.00	3A7
ATOM	827	CB CG	MET MET	145 145	20.243 -33.14		1.00	0.00	3A7
ATOM ATOM	828 829	SD	MET	145	19.496 -33.35		1.00	0.00	3A7
ATOM	830	CE	MET	145	18.314 -31.97		1.00	0.00	3A7
ATOM	831	c	MET	145	20.736 -30.92		1.00	0.00	3A7
ATOM	832	0	MET	145	20.810 -29.70		1.00	0.00	3A7
ATOM	833	N	VAL	146	19.718 -31.60		1.00	0.00	3A7
ATOM	834	CA	VAL	146	18.618 -30.94		1.00	0.00	3A7
MOTA	835	СВ	VAL	146	17.494 -31.86		1.00	0.00	3A7 3A7
ATOM	836		VAL	146	16.290 -30.98 17.145 -32.75		1.00	0.00	3A7
ATOM	837		VAL VAL	146 146	19.066 -30.14		1.00	0.00	3A7
ATOM ATOM	838 839	С 0	VAL	146	18.633 -29.00		1.00	0.00	3A7
ATOM	840	N	PRO	147	19.976 -30.64		1.00	0.00	3A7
ATOM	841	CA	PRO	147	20.491 -29.87		1.00	0.00	3A7
ATOM	842	CD	PRO	147	20.305 -32.06	0 37.960	1.00	0.00	3A7
ATOM	843	CB	PRO	147	21.360 -30.85		1.00	0.00	3A7
ATOM	844	CG	PRO	147	20.726 -32.21		1.00	0.00	3A7
ATOM	845	С	PRO	147	21.286 -28.67		1.00	0.00	3A7 3A7
ATOM	846	0	PRO	147	21.286 -27.68		1.00	0.00	3A7
ATOM	847	N	ILE	148	21.943 -28.72 22.723 -27.63		1.00	0.00	3A7
ATOM	848 849	CA CB	ILE	148 148	23.664 -28.11		1.00	0.00	3A7
ATOM ATOM	850		ILE	148	24.341 -26.92		1.00	0.00	3A7
ATOM	851		ILE	148	24.796 -29.02		1.00	0.00	3A7
ATOM	852	CD	ILE	148	24.460 -30.11		1.00	0.00	3A7 -
ATOM	853	С	ILE	148	21.813 -26.55		1.00	0.00	. 3A7
ATOM	854	0	ILE	148	22.073 -25.36		1.00	0.00	3A7
ATOM	855	N	ILE	149	20.672 -26.90		1.00	0.00	3A7 3A7
ATOM	856	CA	ILE	149	19.682 -26.04		1.00	0.00	3A7
ATOM	857	CB	ILE	149 149	18.645 -26.74 17.595 -25.73		1.00	0.00	3A7
ATOM ATOM	858 859		ILE	149	19.377 -27.39		1.00	0.00	3A7
ATOM	860	CD	ILE	149	18.552 -28.4		1.00	0.00	3A7
ATOM	861	c	ILE	149	19.032 -25.3		1.00	0.00	3A7
ATOM	862	0	ILE	149	18.779 -24.13	36.179	1.00	0.00	3A7
ATOM	863	N	ALA	150	18.793 -26.0		1.00	0.00	3A7
MOTA	864	CA	ALA	150	18.229 -25.4		1.00	0.00	3A7 3A7
MOTA	865	СВ	ALA	150	17.894 -26.5		1.00	0.00	. 3A7
ATOM	866	C	ALA	150 150	19.160 -24.49 18.723 -23.49			0.00	3A7
ATOM	867 868	O N	ALA GLN	151	20.488 -24.7			0.00	3A7
ATOM ATOM	869	CA	GLN	151	21.492 -23.8			0.00	3A7
ATOM	870	СВ	GLN	151	22.910 -24.4			0.00	3A7
ATOM	871	CG	GLN	151	23.192 -25.4		1.00	0.00	3A7
ATOM	872	CD	GLN	151	24.551 -26.1			0.00	3A7
ATOM	873		GLN	151	25.580 -25.4			0.00	3A7 3A7
MOTA	874		GLN	151	24.541 -27.4			0.00	3A7 3A7
MOTA	875	C	GLN	151	21.475 -22.4 21.418 -21.4			0.00	3A7
ATOM	876	0	GLN	151 152	21.418 -21.4			0.00	3A7
ATOM ATOM	877 878	N CA	TYR TYR	152	21.438 -21.2			0.00	3A7
ATOM	879	CB	TYR	152	21.651 -21.5			0.00	3A7
ATOM	880	CG	TYR	152	22.236 -20.2		1.00	0.00	3A7
ATOM	881		TYR	152	23.578 -19.9			0.00	3A7
ATOM	882	CD2	TYR	152	21.411 -19.1			0.00	3A7
MOTA	883		TYR	152	24.053 -18.7			0.00	3A7 3A7
ATOM	884		TYR	152	21.870 -17.8			0.00	3A7
MOTA	885	CZ	TYR		23.208 -17.6 23.690 -16.3			0.00	3A7
ATOM	886 887	OH	TYR TYR		20.140 -20.5			0.00	3A7
ATOM ATOM	888	C O	TYR		20.108 -19.3			0.00	3A7
MOTA	889	N	GLY	153	19.025 -21.3			0.00	3A7
MOTA	890	CA	GLY	153	17.715 -20.7		1.00		3A7
ATOM	891	C	GLY		17.596 -19.9	72 38.59			3A7
MOTA	892	0	GLY		16.977 -18.9	15 38.65	7 1.00	0.00	. 3A7

ATOM	893	N	ASP	154	18.270 -	-20.457	39.650	1.00	0.00		3A7
ATOM	894	ÇA	ASP	154	18.353 -		40.919	1.00	0.00		3A7
MOTA	895	CB	ASP	154	19.017 -		41.976	1.00	0.00		3A7
ATOM	896	CG	ASP	154	18.142 -		42.299	1.00	0.00 0.00		3A7 3A7
ATOM	897	OD1		154 154	16.975 - 18.643 -		41.830 43.039	1.00	0.00		3A7
ATOM	898 899	OD2 C	ASP	154	19.130		40.808	1.00	0.00		3A7
ATOM ATOM	900	ò	ASP	154	18.726 -		41.361	1.00	0.00		3A7
ATOM	901	N	VAL	155	20.243 -		40.041	1.00	0.00		3A7
ATOM	902	CA	VAL	155	21.039 -		39.761	1.00	0.00		3A7
ATOM	903	СВ	VAL	155	22.308 -		38.989	1.00	0.00		3A7 3A7
ATOM	904		VAL	155	23.103 - 23.251 -		38.590 39.870	1.00	0.00		3A7
ATOM ATOM	905 906	CGZ	VAL VAL	155 155	20.273		39.005	1.00	0.00		3A7
ATOM	907	Ö	VAL	155	20.407		39.286	1.00	0.00		3A7
ATOM	908	N	LEU	156	19.427	-16.653	38.035	1.00	0.00		3A7
MOTA	909	CA	LEU	156	18.566		37.295	1.00	0.00		3A7
ATOM	910	СВ	LEU	156	17.791		36.208	1.00	0.00		3A7 3A7
ATOM	911	CG	LEU	156 156	17.040 · 17.539 ·		35.295 33.841	1.00	0.00		3A7
ATOM ATOM	912 913		LEU	156	15.520		35.345	1.00	0.00		3A7
ATOM	914	c	LEU	156	17.570		38.134	1.00	0.00		3A7
ATOM	915	0	LEU	156	17.442		38.081	1.00	0.00		3A7
ATOM	916	N	VAL	157	16.840		38.969	1.00	0.00		3A7 3A7
MOTA	917	CA	VAL	157	15.830 · 15.164 ·		39.861 40.629	1.00	0.00 0.00		3A7
ATOM	918 919	CB	VAL VAL	157 157	14.204		41.728	1.00	0.00		3A7
ATOM ATOM	920		VAL	157	14.373		39.609		0.00		3A7
ATOM	921	c	VAL	157	16.437		40.832	1.00	0.00	•	3A7
MOTA	922	0	VAL	157	15.906		41.069	1.00	0.00		3A7
ATOM	923	N	ARG	158	17.626		41.358	1.00	0.00		3A7 3A7
ATOM	924	CA	ARG	158	18.365 · 19.590 ·		42.251	1.00	0.00		3A7
ATOM ATOM	925 926	CB CG	ARG ARG	158 158	20.308		43.961	1.00	0.00		3A7
ATOM	927	CD	ARG	158	21.475		44.519	1.00	0.00		3A7
ATOM	928	NE	ARG	158	20.932		45.038	1.00	0.00		3A7
ATOM	929	CZ	ARG	158	21.742		45.358	1.00	0.00		3A7 3A7
ATOM	930		ARG	158	21.187 23.097		45.808 45.230	1.00	0.00		3A7
ATOM ATOM	931 932	C	ARG ARG	158 158	18.810		41.638	1.00	0.00		3A7
ATOM	933	ō	ARG	158	18.732		42.274	1.00	0.00		3A7
ATOM	934	N	ASN	159	19.237	-12.550	40.359	1.00	0.00		3A7
MOTA	935	CA	ASN	159	19.621		39.637	1.00	0.00		3A7
ATOM	936	CB	ASN	159	20.171 21.490		38.250 38.358	1.00	0.00		3A7 3A7
ATOM ATOM	937 938	CG	ASN ASN	159 159	22.072		39.439	1.00	0.00		3A7
ATOM	939	ND2		159	21.964		37.177	1.00	0.00		3A7
ATOM	940	С	ASN	159	18.466	-10.408	39.454	1.00	0.00		3A7
MOTA	941	0	ASN.	159		-9.195	39.568	1.00	0.00		3A7
MOTA	942	N	LEU	160	17.267 16.066		39.205 39.031	1.00 1.00	0.00		3A7 3A7
ATOM ATOM	943 944	CA CB	LEU	160 160	14.972		38.383	1.00	0.00		3A7
ATOM	945	CG	LEU	160	15.234		36.902	1.00	0.00		3A7
MOTA	946		LEU	160		-12.430	36.402	1.00	0.00		3A7
ATOM	947		LEU	160		-10.246	35.959	1.00	0.00		3A7
ATOM	948	C	LEU	160	15.557 14.965	-9.655 -8.580	40.349	1.00	0.00		3A7 3A7
ATOM ATOM	949 950	N N	LEU ARG	160 161		-10.377	41.455	1.00	0.00		3A7
ATOM	951	CA	ARG	161	15.487	-9.958	42.787	1.00	0.00		3A7
ATOM	952	CB	ARG	161		-11.052	43.830	1.00	0.00		3A7
ATOM	953	CG	ARG	161		-12.097	43.887	1.00	0.00		3A7
MOTA	954	CD	ARG	161		-13.097	45.047	1.00	0.00		3A7 3A7
ATOM ATOM	955 956	NE CZ	ARG ARG	161 -161		-13.954 -15.051	44.841 45.617	1.00	0.00		3A7
ATOM	957		ARG	161		-15.804	45.374	1.00	0.00		3A7
ATOM	958		ARG	161		-15.400	46.629	1.00	0.00		3A7
MOTA	959	C	ARG	161	16.228	-8.712	43.210	1.00	0.00		3A7
MOTA	960	0	ARG	161	15.673	-7.843 -0.597	43.879	1.00	0.00		3A7 3A7
ATOM ATOM	961 962	N CA	ARG ARG	162 162	17.510 18.380	-8.597 -7.499	42.792 43.134	1.00	0.00		3A7
ATOM	963	CB	ARG	162	19.851	-7.869	42.894	1.00	0.00		3A7
ATOM	964	CG	ARG	162	20.346	-8.986	43.829	1.00	0.00		3A7

ATOM	965	CD	ARG	162	21.838	-9.302	43.666	1.00	0.00	3A7
ATOM	966	NE	ARG	162	22.095	-9.696	42.242	1.00	0.00	3A7
MOTA	967	CZ	ARG	162	23.363	-9.855	41.755	1.00	0.00	3A7
MOTA	968		ARG	162		-10.141	40.433	1.00	0.00	3A7
MOTA	969		ARG	162	24.444	-9.724	42.577	1.00	0.00	3A7 3A7
MOTA	970	C	ARG	162	18.080	-6.236 -5.220	42.355 42.500	1.00	0.00	3A7
ATOM	971	0	ARG	162	18.755 17.014	-5.220	42.500	1.00	0.00	3A7
ATOM	972 973	N CA	GLU	163 163	16.615	-5.103	40.744	1.00	0.00	3A7
ATOM ATOM	974	CB	GLU	163	15.965	-5.504	39.413	1.00	0.00	3A7
ATOM	975	CG	GLU	163	16.981	-6.330	38.605	1.00	0.00	3A7
ATOM	976	CD	GLU	163	16.426	-6.716	37.246	1.00	0.00	3A7
ATOM	977		GLU	163	17.080	-6.372	36.227	1.00	0.00	3A7
ATOM	978	OE2	GLU	163	15.354	-7.376	37.210	1.00	0.00	3A7
MOTA	979	С	GLU	163	15.784	-4.183	41.582	1.00	0.00	3A7
ATOM	980	0	GLU	163	15.662	-2.998	41.288	1.00	0.00	3A7
MOTA	981	N	ALA	164	15.230	-4.708	42.699	1.00	0.00	3A7 3A7
ATOM	982	CA	ALA	164	14.728	-3.939	43.812	1.00	0.00	3A7
ATOM	983	CB	ALA	164	15.779	-2.963 -3.200	44.394 43.529	1.00	0.00	3A7
ATOM	984	C	ALA	164 164	13.480 13.505	-1.993	43.525	1.00	0.00	3A7
ATOM ATOM	985 986	о И	ALA GLU	165	12.363	-3.878	43.176	1.00	0.00	3A7
ATOM	987	CA	GLU	165	10.993	-3.400	43.222	1.00	0.00	3A7
MOTA	988	СВ	GLU	165	10.561	-2.688	44.540	1.00	0.00	3A7
ATOM	989	CG	GLU	1.65	10.851	-3.510	45.809	1.00	0.00	3A7
MOTA	990	CD	GLU		10.308	-2.803	47.050	1.00	0.00	3A7
MOTA	991	OE1	GLU	165	9.757	-1.678	46.915	1.00	0.00	3A7
ATOM	992	OE2	GLU	165	10.441	-3.390	48.158	1.00	0.00	3A7
ATOM	993	С	GLU	165	10.541	-2.574	42.031	1.00	0.00	3A7
MOTA	994	0	GLU	165	9.403	-2.728	41.595	1.00	0.00	3A7
MOTA	995	N	THR	166	11.382	-1.661	41.488	1.00	0.00	3A7 3A7
ATOM	996	CA	THR	166 166	10.979 10.351	-0.758 0.509	40.425 40.932	1.00	0.00	3A7
ATOM ATOM	997 998	CB	THR	166	9.175	0.217	41.676	1.00	0.00	3A7
ATOM	999	CG2	THR	166	9.944	1.442	39.767	1.00	0.00	3A7
ATOM	1000	c	THR	166	12.235	-0.374	39.728	1.00	0.00	3A7
ATOM	1001	o	THR	166	12.410	-0.652	38.547	1.00	0.00	3A7
ATOM	1002	N	GLY	167	13.141	0.230	40.560	1.00	0.00	3A7
ATOM	1003	CA	GLY	167	14.556	0.524	40.415	1.00	0.00	3A7
MOTA	1004	С	GLY	167	14.980	0.965	39.058	1.00	0.00	3A7
ATOM	1005	0	GLY	167	15.037		38.750	1.00	0.00	3A7 3A7
ATOM	1006	N	LYS	168	15.246	-0.048	38.208 36.801	1.00	0.00	3A7
ATOM	1007 1008	CA CB	LYS LYS	168 168	15.423 16.887	0.121	36.380	1.00	0.00	3A7
ATOM ATOM	1008	CG	LYS	168	17.309	0.475	35.050	1.00	0.00	3A7
ATOM	1010	CD	LYS	168	18.803	0.294	34.725	1.00	0.00	3A7
ATOM	1011	CE	LYS	168	19.236	-1.160	34.483	1.00	0.00	3A7
ATOM	1012	NZ	LYS	168	18.558	-1.731	33.297	1.00	0.00	3A7
ATOM	1013	Ċ	LYS	168	14.438	-0.857	36.181	1.00	0.00	. 3A7
ATOM	1014	0	LYS	168	14.315	-1.969	36.694	1.00	0.00	3A7
MOTA	1015	N	PRO	169	13.751	-0.544	35.061	1.00	0.00	3A7
ATOM	1016	CA	PRO	169	13.228	-1.488	34.077	1.00	0.00	3A7 3A7
ATOM	1017	CD	PRO	169	13.706	0.834	34.565	1.00	0.00	3A7
ATOM	1018	CB	PRO	169 169	12.639 13.438	-0.568 0.725	33.005 33.072	1.00	0.00	3A7
ATOM ATOM	1019	CC	PRO PRO	169	14.386	-2.289	33.508	1.00	0.00	3A7
ATOM	1021	ō	PRO	169	15.533	-1.866	33.608	1.00	0.00	3A7
ATOM	1022	N	VAL	170	14.110	-3.480	32.963	1.00	0.00	3A7
ATOM	1023	CA	VAL	170	15.120	-4.462	32.688	1.00	0.00	3A7
MOTA	1024	CB	VAL	170	14.791	-5.773	33.379	1.00	0.00	3A7
MOTA	1025	CG1	VAL	170	15.992	-6.742	33.323	1.00	0.00	3A7
ATOM	1026		VAL	170	14.350	-5.485	34.825	1.00	0.00	3A7
MOTA	1027	C	VAL	170	15.190	-4.659	31.200	1.00	0.00	3A7
ATOM	1028	0	VAL	170	14.185	-4.556	30.501	1.00	0.00	3A7 3A7
ATOM	1029	N	THR	171	16.400	-4.984 -5.364	30.690 29.321	1.00	0.00	3A7
MOTA	1030	CA CB	THR THR	171 171	16.616 17.889	-5.364 -4.784	29.321	1.00	0.00	3A7
MOTA MOTA	1031 1032		THR	171	17.858	-3.368	28.857	1.00	0.00	3A7
ATOM	1032		THR	171	18.018	-5.145	27.233	1.00	0.00	3A7
ATOM	1034	c	THR	171	16.717	-6.854	29.319	1.00	0.00	3A7
ATOM	1035	ŏ	THR	171	17.667	-7.434	29.839	1.00	0.00	3A7
ATOM	1036	N	LEU	172	15.716	-7.527	28.719	1.00	0.00	3A7

ATOM	1037	CA	LEU	172	15.566	-8.955	28.820	1.00	0.00	3A7
ATOM	1038	СВ	LEU	172	14.147	-9.409	28.421	1.00	0.00	3A7
ATOM	1039	CG	LEU	172	12.958	-8.735	29.139	1.00	0.00	3A7
ATOM	1040	CD1	LEU	172	13.118	-8.664	30.670	1.00	0.00	3A7
ATOM	1041	CD2	LEU	172	12.633	-7.378	28.501	1.00	0.00	3A7
ATOM	1042	С	LEU	172	16.574	-9.705	27.991	1.00	0.00	3A7
MOTA	1043	0	LEU	172			28.384	1.00	0.00	3A7
MOTA	1044	N	LYS	173	16.994	-9.161	26.826	1.00	0.00	3A7 3A7
ATOM	1045	CA	LYS	173	17.961	-9.803	25.952 24.685	1.00	0.00	3A7
ATOM	1046	CB	LYS LYS	173 173	18.202 19.033	-8.967 -9.687	23.605	1.00	0.00	3A7
MOTA MOTA	1047 1048	CG CD	LYS	173	19.257	-8.825	22.357	1.00	0.00	3A7
ATOM	1049	CE	LYS	173	19.931	-9.589	21.211	1.00	0.00	3A7
ATOM	1050	NZ	LYS	173	20.065	-8.725	20.017	1.00	0.00	3A7
ATOM	1051	C.	LYS	173		-10.057	26.620	1.00	0.00	3A7
ATOM	1052	0	LYS	173	19.912	-11.106	26.445	1.00	0.00	3A7
ATOM	1053	N	HIS	174	19.729	-9.103	27.472	1.00	0.00	3A7
MOTA	1054	CA	HIS	174	20.962	-9.190	28.204	1.00	0.00	3A7
ATOM	1055		HIS	174	23.840	-7.893	28.844	1.00	0.00	3A7 3A7
ATOM	1056	CG	HIS	174	22.644	-7.783	29.521	1.00	0.00	3A7
ATOM	1057	CB	HIS	174	21.288 24.347	-7.846 -7.664	28.865 30.996	1.00	0.00	3A7
ATOM	1058 1059		HIS	174 174	22.973	-7.645	30.834	1.00	0.00	3A7
ATOM ATOM	1060		HIS	174	24.824	-7.814	29.775	1.00	0.00	3A7
ATOM	1061	CEI	HIS	174		-10.255	29.275	1.00	0.00	3A7
ATOM	1062	ŏ	HIS	174		-11.082	29.317	1.00	0.00	3A7
ATOM	1063	N	VAL	175	19.954	-10.272	30.170	1.00	0.00	3A7
ATOM	1064	CA	VAL	175	19.876	-11.181	31.303	1.00	0.00	3A7
ATOM	1065	СВ	VAL	175		-10.715	32.291	1.00	0.00	3A7
MOTA	1066		VAL	175		-11.586	33.568	1.00	0.00	3A7
ATOM	1067		VAL	175	19.117	-9.239	32.645	1.00	0.00	3A7
ATOM	1068	C	VAL	175		-12.603	30.872	1.00	0.00	3A7 3A7
ATOM	1069	0	VAL	175		-13.576	31.455 29.799	1.00	0.00	3A7
ATOM	1070	N	PHE	176 176		-12.751 -14.047	29.302	1.00	0.00	3A7
MOTA MOTA	1071 1072	CA CB	PHE	176		-13.978	28.573	1.00	0.00	3A7
ATOM	1072	CG	PHE	176		-14.019	29.651	1.00	0.00	3A7
ATOM	1074		PHE	176		-12.887	30.048	1.00	0.00	3A7
ATOM	1075		PHE	176		-15.216	30.337	1.00	0.00	3A7
ATOM	1076	CE1	PHE	176	14.380	-12.941	31.117	1.00	0.00	3A7
ATOM	1077	CE2	PHE	176		-15.282	31.394	1.00	0.00	3A7
ATOM	1078	CZ	PHE	176		-14.139	31.790	1.00	0.00	3A7
ATOM	1079	C	PHE	176		-14.648	28.382	1.00	0.00	3A7 3A7
MOTA	1080		. PHE	176		-15.860	28.180 27.829	1.00	0.00	3A7
ATOM	1081 1082	N CA	GLY	177 177		-13.824 -14.314	27.061	1.00	0.00	3A7
ATOM ATOM	1082	C	GLY	177		-14.791	27.997	1.00	0.00	3A7
ATOM	1084	ŏ	GLY	177		-15.756	27.714	1.00	0.00	3A7
ATOM	1085	N	ALA	178		-14.142	29.180	1.00	0.00	3A7
ATOM	1086	CA	ALA	178	23.616	-14.483	30.214	1.00	0.00	3A7
ATOM	1087	СВ	ALA	178		-13.426	31.327	1.00	0.00	3A7
MOTA	1088	С	ALA	178		-15.805	30.855	1.00	0.00	3A7
ATOM	1089	0	ALA	178		-16.635	31.070	1.00	0.00	3A7 3A7
ATOM	1090	N	TYR	179		-16.063	31.127 31.732	1.00	0.00	3A7
ATOM ATOM	1091	CA CB	TYR	179		-17.288 -17.174	31.732	1.00	0.00	3A7
ATOM	1092 1093	CG	TYR TYR	179 179		-18.432	31.952	1.00	0.00	3A7
ATOM	1094		TYR	179		-18.892	33.140	1.00	0.00	3A7
ATOM	1095		TYR	179		-19.133	30.778	1.00	0.00	3A7
ATOM	1096		TYR	179		-20.112	33.200	1.00	0.00	3A7
ATOM	1097		TYR	179		-20.354	30.824	1.00	0.00	3A7
MOTA	1098	CZ	TYR	179		-20.868	32.046		0.00	3A7
MOTA	1099	ОН	TYR	179		-22.143	32.117	1.00	0.00	3A7
MOTA	1100	С	TYR	179		-18.504	30.914	1.00	0.00	3A7
MOTA	1101	0	TYR	179		-19.487	31.413	1.00	0.00	3A7
ATOM	1102	N	SER	180		-18.432	29.602	1.00	0.00	3A7 3A7
ATOM	1103	CA	SER	180		-19.553 -19.328	28.719 27.464	1.00	0.00	3A7
ATOM ATOM	1104 1105	CB OG	SER SER	180 180		-19.328	26.860	1.00	0.00	3A7
ATOM	1105	c	SER	180		-19.852	28.402	1.00	0.00	3A7
ATOM	1107	ŏ	SER	180		-21.010	28.278	1.00	0.00	3A7
MOTA	1108	N	MET	181		-18.834	28.319	1.00	0.00	3A7

ATOM	1109	CA	MET	181	25.507	-19.052	28.132	1.00	0.00	3A7
ATOM	1110	CB	MET	181	26.246		27.978	1.00	0.00	3A7
ATOM	1111	CG	MET	181	25.986		26.568 26.130	1.00	0.00	3A7 3A7
ATOM ATOM	1112 1113	SD CE	MET MET	181 181	26.894 25.919		27.203	1.00	0.00	3A7
ATOM	1114	C	MET	181	26.127		29.282	1.00	0.00	3A7
ATOM	1115	Ō	MET	181	26.923		29.117	1.00	0.00	3A7
ATOM	1116	N	ASP	182	25.695		30.493	1.00	0.00	3A7 3A7
ATOM	1117	CA	ASP ASP	182 182	26.174 25.809		31.695 32.908	1.00	0.00	3A7
ATOM ATOM	1118 1119	CB CG	ASP	182	26.545		32.877	1.00	0.00	3A7
ATOM	1120		ASP	182	27.380	-17.590	31.961	1.00	0.00	3A7
MOTA	1121		ASP	182	26.276		33.788	1.00	0.00	3A7 3A7
ATOM	1122	C	ASP	182 182	25.645 26.371		31.886 32.382	1.00	0.00	3A7
MOTA MOTA	1123 1124	N O	ASP VAL	183	24.401		31.448	1.00	0.00	3A7
ATOM	1125	CA	VAL	183	23.887		31.514	1.00	0.00	3A7
MOTA	1126	СВ	VAL	183	22.419		31.124	1.00	0.00	3A7
ATOM	1127		VAL	183	21.919 21.578		30.984 32.200	1.00	0.00	3A7 3A7
ATOM ATOM	1128 1129	CG2	VAL VAL	183 183	24.678		30.610	1.00	0.00	3A7
MOTA	1130	ŏ	VAL	183	25.065		31.027	1.00	0.00	3A7
ATOM	1131	N	ILE	184	24.999		29.353	1.00	0.00	3A7
MOTA	1132	CA	ILE	184	25.762		28.439	1.00	0.00	3A7 3A7
ATOM .	1133	CB	ILE	184 184	25.800 26.594		27.039 26.093	1.00	0.00	3A7
ATOM ATOM	1134 1135		ILE	184	24.365		26.489	1.00	0.00	3A7
ATOM	1136	CD	ILE	184	23.531	-24.898	26.404	1.00	0.00	3A7
ATOM	1137	С	ILE	184	27.167		28.928	1.00	0.00	3A7 3A7
MOTA	1138	0	ILE.		27.720 27.774		28.859 29.486	1.00	0.00	3A7
ATOM ATOM	1139 1140	N CA	THR THR	185 185	29.125		30.002	1.00	0.00	3A7
ATOM	1141	СВ	THR	185	29.617		30.359	1.00	0.00	3A7
MOTA	1142		THR	185	29.625		29.187	1.00	0.00	3A7
MOTA	1143		THR	185	31.047		30.943 31.192	1.00 1.00	0.00	3A7 3A7
ATOM ATOM	1144 1145	C O.	THR THR	185 185	29.259 30.220	-25.166	31.343	1.00	0.00	3A7
ATOM	1146	N	SER	186	28.242		32.066	1.00	0.00	3A7
ATOM	1147	CA	SER	186		-25.188	33.262	1.00	0.00	3A7
ATOM	1148	CB	SER	186		-24.719 -23.412	34.259 34.719	1.00	0.00	3A7 3A7
ATOM -	1149 1150	OG C	SER SER	186 186		-26.655	33.000	1.00	0.00	3A7
ATOM	1151	ŏ	SER	186		-27.500	33.598	1.00	0.00	3A7
MOTA	1152	N	THR	187		-27.006	32.060	1.00	0.00	3A7
MOTA		CA	THR	187		-28.386	31.711	1.00	0.00	3A7 3A7
ATOM ATOM	1154 1155	CB OG1	THR.	187 187		-28.580 -27.748	30.943 29.789	1.00	0.00	3A7
ATOM	1156		THR	187		-28.285	31.861	1.00	0.00	3A7
ATOM	1157	С	THR	187 .		-28.983	30.897	1,00	0.00	3A7
MOTA	1158	0	THR	187		-30.195	30.899	1.00	0.00	. 3A7 3A7
MOTA MOTA	1159 1160	N CA	SER SER	188 188		-28.115 -28.556	30.176 29.280	1.00	0.00	3A7
ATOM	1161	СВ	SER	188		-27.697	27.991	1.00	0.00	- 3A7
MOTA	1162	OG	SER	188	30.272	-26.347	28.250		0.00	3A7 ·
ATOM	1163	С	SER	188		-28.690	29.970	1.00	0.00	3A7 3A7
ATOM ATOM	1164 1165	O N	SER PHE	188 189		-29.681 -27.672	29.768 30.766	1.00	0.00	3A7
ATOM	1166	CA	PHE	189		-27.581	31.256	1.00	0.00	3A7
ATOM	1167	СВ	PHE	189	33.653	-26.363	30.732	1.00	0.00	3A7
ATOM	1168	CG	PHE	189		-26.027	29.300	1.00	0.00	3A7 3A7
ATOM	1169 1170		PHE	189 189		-24.694 -26.986	28.976 28.292	1.00	0.00	3A7
ATOM ATOM	1171		PHE	189		-24.317	27.665	1.00	0.00	3A7
ATOM	1172		PHE	189	33.182	-26.618	26.984	1.00	0.00	3A7
ATOM	1173	cz	PHE	189		-25.284	26.668	1.00	0.00	3A7 3A7
ATOM	1174	C	PHE	189 189		-27.463 -27.441	32.762 33.361	1.00	0.00	3A7
ATOM ATOM	1175 1176	O N	PHE GLY	190		-27.378	33.435	1.00	0.00	3A7
ATOM	1177	CA	GLY	190	31.654	-27.345	34.883	1.00	0.00	3A7
MOTA	1178	С	GLY	190		-25.956	35.418	1.00	0.00	3A7
ATOM ATOM	1179 1180	O N	GLY VAL	190 191		-25.095 -25.744	35.280 36.044	1.00	0.00	3A7 3A7
ALL LAT	1100	1.4	VAL	171	JJ. UJ/					-···

ATOM	1181	CA	VAL	191	33.597	-24.510	36.596	1.00	0.00	3A7
ATOM	1182	СВ	VAL	191		-23.250	35.727	1.00	0.00	3A7
MOTA	1183	CG1		191		-22.372	36.078	1.00	0.00	3A7
MOTA	1184	CG2		191		-22.424 -24.310	35.812 38.012	1.00	0.00	3A7 3A7
ATOM	1185	C	VAL VAL	191 191		-24.510 -24.551	38.325	1.00	0.00	3A7
ATOM ATOM	1186 1187	O N	SER	192		-23.844	38.900	1.00	0.00	3A7
ATOM	1188	CA	SER	192		-23.531	40.281	1.00	0.00	3A7
ATOM	1189	СВ	SER	192		-24.116	41.252	1.00	0.00	3A7
ATOM	1190	OG	SER	192		-25.534	41.156	1.00	0.00	3A7 3A7
MOTA	1191	C	SER	192 192		-22.032 -21.317	40.410 39.501	1.00	0.00	3A7
ATOM ATOM	1192 1193	N O	SER	193		-21.524	41.572	1.00	0.00	3A7
ATOM	1194	CA	ILE	193		-20.109	41.867	1.00	0.00	3A7
MOTA	1195	CB .	ILE	193		-19.756	42.671	1.00	0.00	3A7
MOTA	1196		ILE	193		-18.225	42.861	1.00	0.00	3A7
MOTA	1197		ILE	193		-20.322 -19.784	41.992 40.581	1.00	0.00	3A7 3A7
ATOM ATOM	1198 1199	CD C	ILE	193 193		-19.720	42.618	1.00	0.00	3A7
ATOM	1200	ò	ILE	193		-19.967	43.816	1.00	0.00	3A7
ATOM	1201	N	ASP	194	35.344	-19.102	41.887	1.00	0.00	3A7
ATOM	1202	CA	ASP	194		-18.685	42.420	1.00	0.00	3A7
ATOM	1203	CB	ASP	194		-19.786	42.267	1.00	0.00	3A7 3A7
ATOM ATOM	1204	CG	ASP ASP	194 194		-19.433 -19.270	43.034 44.280	1.00 1.00	0.00	3A7
ATOM	1205 1206		ASP	194		-19.326	42.381	1.00	0.00	3A7
MOTA	1207.	c	ASP	194		-17.442	41.654	1.00	0.00	3A7
MOTA	1208	0	ASP	194		-16.608	42.141	1.00	0.00	3A7
ATOM	1209	N	SER	195		-17.299	40.420	1.00	0.00	3A7 3A7
ATOM	1210 1211	CA	SER	195 195		-16.163 -16.561	39.548 38.055	1.00	0.00	3A7
ATOM ATOM	1211	CB OG	SER	195		-17.464	37.811	1.00	0.00	3A7
ATOM	1213	c	SER	195		-15.185	39.763	1.00	0.00	3A7
ΛΤΟΜ	1214	0	SER	195		-15.547	40.256	1.00	0.00	3A7
ATOM	1215	N	LEU	196		-13.902	39.386	1.00	0.00	3A7 3A7
ATOM	1216 1217	CA CB	LEU	196 196		-12.813 _. -11.523	39.580 40.138	1.00	0.00	3A7
ATOM ATOM	1217	·CG	LEU	196		-11.639	41.551	1.00	0.00	3A7
ATOM	1219		LEU	196		-12.190	42.599	1.00	0.00	3A7
ATOM	1220		LEU	196		-12.399	41.574	1.00	0.00	3A7
MOTA	1221	С	LEU	196		-12.481	38.258	1.00	0.00	3A7 3A7
ATOM ATOM	1222 1223	O N	LEU ASN	196 197		-11.334 -13.503	38.022 37.366	1.00	0.00	3A7
ATOM	1224	ÇA	ASN	197		-13.455	36.068	1.00	0.00	3A7
ATOM	1225	СВ	ASN	197		-12.846	36.138	1.00	0.00	3A7
ATOM	1226	CG	ASN	197		-13.111	34.865	1.00	0.00	3A7
ATOM	1227		ASN	197		-14.206	34.295	1.00	0.00	3A7 3A7
ATOM	1228 1229	ND2	ASN ASN	197 197		-12.069 -12.714	34.431 35.072	1.00	0.00	3A7
ATOM ATOM	1230	Ö	'ASN	197		-11.770	34.419	1.00	0.00	3A7
ATOM	1231	N	ASN	198		-13.134	34.960	1.00	0.00	. 3A7
MOTA	1232	CA	ASN	198		-12.476	34.117	1.00	0.00	3A7
ATOM	1233	CB	ASN	198		-12.191	34.815 36.121	1.00	0.00	3A7 3A7
ATOM ATOM	1234 1235	CG OD1	ASN ASN	198 198		-11.423 -11.949	37.214	1.00	0.00	3A7
ATOM	1236		ASN	198		-10.153	35.986	1.00	0.00	3A7
ATOM	1237	С	ASN	198	36.725	-13.246	32.825	1.00	0.00	3A7
MOTA	1238	0	ASN	198		-12.598	31.789	1.00	0.00	3A7
ATOM	1239	N	PRO	199		-14.562	32.735 31.473	1.00	0.00	3A7 3A7
MOTA MOTA	1240 1241	CA CD	PRO PRO	199 199		-15.242 -15.415	33.865	1.00	0.00	3A7
ATOM	1241	CB	PRO	199		-16.553	31.866	1.00	0.00	3A7
ATOM	1243	CG	PRO	199	38.421	-16.338	33.313	1.00	0.00	3A7
ATOM	1244	С	PRO	199		-15.538	30.731	1.00	0.00	3A7
ATOM	1245	0	PRO	199		-15.766	29.524 31.441	1.00	0.00	3A7 3A7
MOTA MOTA	1246 1247	N CA	GLN GLN	200 200		-15.560 -15.967	30.914	1.00	0.00	3A7
MOTA	1247	CB	GLN	200		-16.559	32.023	1.00	0.00	3A7
MOTA	1249	CG	GLN	200	31.297	-17.173	31.515	1.00	0.00	3A7
MOTA	1250	CD	GLN	200		-17.885	32.668	1.00	0.00	3A7
MOTA	1251		GLN	200		-19.110	32.645	1.00	0.00	3A7 3A7
MOTA	1252	NE2	GLN	200	30.150	-17.085	33.690	1.00	0.00	3A /

ATOM	1253	С	GLN	200	32.815	-14.819	30.232	1.00	0.00	3A7
		ō	GLN	200		-15.035	29.233	1.00	0.00	3A7
ATOM	1254					-13.568	30.743	1.00	0.00	3A7
ATOM	1255		ASP	201				1.00	0.00	3A7
ATOM	1256	CA	ASP	201		-12.384	30.219			
ATOM	1257	CB	ASP	201		-11.254	31.288	1.00	0.00	3A7
ATOM	1258	CG	ASP	201	31.197	-10.174	30.927	1.00	0.00	3A7
ATOM	1259	ODI	ASP	201	31.610	-8.994	30.772	1.00	0.00	3A7
ATOM	1260		ASP	201	29, 992	-10.520	30.805	1.00	0.00	3A7
			ASP	201		-11.859	28.899	1.00	0.00	3A7
ATOM	1261	C					28.095	1.00	0.00	3A7
ATOM	1262	0	ASP	201		-11.342			0.00	3A7
ATOM	1263	N	PRO	202		-11.966	28.590	1.00		
ATOM	1264	CA	PRO	202	34.768	-11.731	27.282	1.00	0.00	3A7
ATOM	1265	CD	PRO	202	35.191	-11.898	29.612	1.00	0.00	3A7
ATOM	1266	СВ	PRO	202	36.280	-11.790	27.543	1.00	0.00	3A7
ATOM	1267	CG	PRO	202	36.411	-11.259	28.958	1.00	0.00	3A7
ATOM	1268	C	PRO	. 202	34.334	-12.755	26.270	1.00	0.00	3A7
			PRO	202		-12.386	25.126	1.00	0.00	3A7
MOTA	1269	0					26.662	1.00	0.00	3A7
ATOM	1270	N	PHE	203		-14.041			0.00	3A7
MOTA	1271	CA	PHE	203		-15.113	25.807	1.00		
ATOM	1272	СВ	PHE	203		-16.402	26.628	1.00	0.00	3A7
ATOM	1273	CG	PHE	203	33.530	-17.655	25.800	1.00	0.00	3A7
ATOM	1274	CD1	PHE	203	34.701	-18.401	25.685	1.00	0.00	3A7
ATOM	1275		PHE	203	32.364	-18.126	25.192	1.00	0.00	3A7
	1276		PHE	203		-19.599	24.981	1.00	0.00	3A7
ATOM						-19.316	24.471	1.00	0.00	3A7
MOTA	1277		PHE	203					0.00	3A7
MOTA	1278	CZ	PHE	203		-20.060	24.377	1.00		
ATOM	1279	С	PHE	203		-14.780	25.173	1.00	0.00	3A7
ATOM	1280	0	PHE	203	32.125	-15.040	23.999	1.00	0.00	3A7
ATOM	1281	N	VAL	204	31.455	-14.147	25.959	1.00	0.00	3A7
ATOM	1282	CA	VAL	204	30.141	-13.686	25.564	1.00	0.00	3A7
ATOM	1283	СВ	VAL	204		-12.914	26.710	1.00	0.00	3A7
ATOM	1284		VAL	204		-12.240	26.286	1.00	0.00	3A7
						-13.845	27.927	1.00	0.00	3A7
ATOM	1285		VAL	204						3A7
ATOM	1286	С	VAL	204		-12.702	24.430	1.00	0.00	
ATOM	1287	0	VAL	204		-12.835	23.424	1.00	0.00	3A7
ATOM	1288	N	GLU	205	31.077	-11.674	24.576	1.00	0.00	3A7
ATOM	1289	CA	GLU	205	31.235	-10.607	23.617	1.00	0.00	3A7
ATOM	1290	СВ	GLU	205	32.215	-9.544	24.146	1.00	0.00	3A7
ATOM	1291	CG	GLU	205	32.242	-8.242	23.327	1.00	0.00	3A7
ATOM	1292	CD	GLU	205	33.217		23.979	1.00	0.00	3A7
	1293		GLU	205	32.974	-6.880	25.153	1.00	0.00	3A7
ATOM								1.00	0.00	3A7
ATOM	1294		GLU	205	34.219		23.310			3A7
ATOM	1295	C	GLU	205		-11.106	22.289	1.00	0.00	
MOTA	1296	0	GLU	205		-10.646	21.238	1.00	0.00	3A7
ATOM	1297	N	ASN	206		-12.123	22.316	1.00	0.00	3A7
ATOM	1298	CA	ASN	206	33.175	-12.741	21.134	1.00	0.00	3A7
ATOM	1299	СВ	ASN	206	34.358	-13.657	21.467	1.00	0.00	. 3A7
ATOM	1300	CG	ASN	206	35,509	-12.819	22.025	1.00	0.00	3A7
ATOM	1301		ASN	206		-12.848	23.224	1.00	0.00	3A7
	1302	-	ASN	206		-12.023	21.120	1.00	0.00	3A7
ATOM							20.380	1.00	0.00	3A7
ATOM	1303	C	ASN	206		-13.539				3A7
ATOM	1304	0	ASN	206		-13.337	19.182	1.00	0.00	
ATOM	1305	N	THR	207		-14.452	21.067	1.00	0.00	3A7
ATOM	1306	CA	THR	207		-15.301	20.464	1.00	0.00	3A7
ATOM	1307	CB	THR	207	29.749	-16.188	21.502	1.00	0.00	3A7
ATOM	1308		THR	207	30.751	-16.917	22.199	1.00	0.00	3A7
ATOM	1309		THR	207		-17.201	20.851	1.00	0.00	3A7
ATOM	1310	c	THR	207		-14.492	19.768	1.00	0.00	3A7
						-14.790		1.00	0.00	3A7
ATOM	1311	0	THR	207			18.646			3A7
MOTA	1312	N	LYS	208		-13.379	20.411	1.00	0.00	
MOTA	1313	CA	LYS	208		-12.459	19.890	1.00	0.00	3A7
ATOM	1314	СВ	LYS	208		-11.413	20.954	1.00	0.00	3A7
MOTA	1315	CG	LYS	208	26.398	-10.524	20.601	1.00	0.00	3A7
ATOM	1316	CD	LYS	208	25.914	-9.608	21.741	1.00	0.00	3A7
ATOM	1317	CE	LYS	208	26.801		22.018	1.00	0.00	3A7
ATOM	1318	NZ	LYS	208	28.077		22.673	1.00	0.00	3A7
						-11.760	18.619	1.00	0.00	3A7
ATOM	1319	C	LYS	208					0.00	3A7
ATOM	1320	0	LYS	208		-11.653	17.675	1.00		
MOTA	1321	N	LYS	209		-11.316	18.536	1.00	0.00	3A7
MOTA	1322	CA	LYS	209		-10.686	17.348	1.00	0.00	3A7
ATOM	1323	CB	LYS	209	31.622	-10.129	17.587	1.00	0.00	3A7
MOTA	1324	CG	LYS	209	31.660	-8.877	18.478	1.00	0.00	3A7
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ATOM	1325	CD	LYS	209	33.007	-8.133	18.418	1.00	0.00		3A7
ATOM	1326	CE	LYS	209	34.227	-8.963	18.843	1.00	0.00		3A7
ATOM	1327	NZ	LYS	209	34.144	-9.343	20.270	1.00	0.00		3A7 3A7
ATOM	1328	C	LYS	209	30.275 29.942		16.153 15.031	1.00	0.00		3A7
ATOM	1329	O N	LYS Leu	209 210	30.662		16.376	1.00	0.00		3A7
ATOM ATOM	1330 1331	CA	LEU	210	30.592		15.391	1.00	0.00		3A7
ATOM	1332	СВ	LEU	210	30.985		16.011	1.00	0.00		3A7
ATOM	1333	CG	LEU	210	31.127		15.108	1.00	0.00		3A7
MOTA	1334		LEU	210	31.072		16.013	1.00	0.00		3A7 3A7
ATOM	1335		LEU	210	30.134 29.217		13.954 14.809	1.00	0.00		3A7
ATOM ATOM	1336 1337	С 0	LEU	210 210	29.056		13.595	1.00	0.00		3A7
ATOM	1338	N	LEU	211	28.185		15.680	1.00	0.00		3A7
ATOM	1339	CA	LEU	211	26.814	-14.406	15.302	1.00	0.00		3A7
ATOM	1340	CB	LEU	211		-14.273	16.480	1.00	0.00		3A7
MOTA	1341	CG	LEU	211		-15.159	17.726	1.00	0.00		3A7 3A7
MOTA	1342		LEU	211 211	26.398	-15.056 -16.614	18.669 17.396	1.00	0.00		3A7
ATOM ATOM	1343 1344	C	LEU	211		-13.442	14.274	1.00	0.00		3A7
ATOM	1345	ŏ	LEU	211		-13.847	13.418	1.00	0.00		3A7
ATOM	1346	N	ARG	212		-12.140	14.324	1.00	0.00		3A7
MOTA	1347	CA	ARG	212		-11.136	13.386	1.00	0.00		3A7
ATOM	1348	СВ	ARG	212	25.985	-9.737	14.028 14.927	1.00	0.00		3A7 3A7
ATOM	1349	CG	ARG	212 212	27.103 28.270	-9.170 -8.508	14.183	1.00	0.00		3A7
ATOM ATOM	1350 1351	CD NE	ARG ARG	212	29.078	-7.724	15.175	1.00	0.00		3A7
ATOM	1352	cz	ARG	212	30.393	-7.406	14.970	1.00	0.00		3A7
ATOM	1353		ARG	212	31.075	-7.901	13.898	1.00	0.00		3A7
ATOM	1354	NH2	ARG	212	31.031	-6.581	15.851	1.00	0.00		3A7
ATOM	1355	C	ARG	212		-11.091	12.169 12.272	1.00	0.00		3A7 3A7
ATOM	1356	O N	ARG PHE	212 213		-11.083 -11.117	10.976	1.00	0.00		3A7
ATOM ATOM	1357 1358	CA	PHE	213		-11.263	9.611	1.00	0.00		3A7
ATOM	1359	СВ	PHE	213	27.428	-9.944	8.921	1.00	0.00		3A7
ATOM	1360	CG	PHE	213	28.597	-9.221	9.541	1.00	0.00		3A7
MOTA	1361		PHE	213	28.391	-8.264	10.535	1.00	0.00		3A7 3A7
MOTA	1362		PHE	213	29.890 29.455	-9.399 -7.517	9.039 11.032	1.00	0.00		3A7
ATOM ATOM	1363 1364		PHE	213 213	30.959	-8.666	9.546	1.00	0.00		3A7
ATOM	1365	CZ	PHE	213	30.741	-7.723	10.544	1.00	0.00		3A7
ATOM	1366	C	PHE	213	27.926	-12.408	9.426	1.00	0.00		3A7
MOTA	1367	0	PHE	213		-12.215	9.209	1.00	0.00		3A7
ATOM	1368	N	ASN	214		-13.649	9.491 9.165	1.00	0.00		3A7 3A7
. ATOM ATOM	1369 1370	CA CB	ASN ASN	214 214		-14.839 -15.372	10.314	1.00	0.00		3A7
ATOM	1371	CG	ASN	214		-16.484	9.818	1.00	0.00		3A7
ATOM	1372		ASN	214		-16.242	8.972	1.00	0.00		3A7
ATOM	1373	ND2	ASN	214		-17.720	10.370	1.00	0.00		3A7
ATOM	1374	Ç	ASN	214		-15.863	8.671	1.00	0.00		3A7 3A7
MOTA	1375	N O	ASN	214 215		-16.351 -16.260	7.565 9.344	1.00	0.00	•	3A7
MOTA MOTA	1376 1377	CA	PRO PRO	215		-17.305	8.858	1.00	0.00		3A7
ATOM	1378	CD	PRO	215		-15.929	10.728	1.00	0.00		3A7
ATOM	1379	CB	PRO	215		-17.865	10.125	1.00	0.00		3A7
MOTA	1380	CG	PRO	215		-17.241	11.310	1.00	0.00		3A7 3A7
ATOM	1381	C	PRO	215		-16.681 -15.982	7.893 8.353	1.00	0.00		3A7
ATOM ATOM	1382 1383	О. И	PRO LEU	215 216		-16.921	6.560	1.00	0.00		3A7
ATOM	1384	CA	LEU	216		-16.424	5.463	1.00	0.00		3A7
ATOM	1385	СВ	LEU	216		-16.737	5.575	1.00	0.00		3A7
ATOM	1386	CG	LEU	216		-18.224	5.393	1.00	0.00		3A7
MOTA	1387		LEU	216		-18.782	4.017	1.00	0.00		3A7 3A7
ATOM	1388 1389		LEU	216 216		-19.148 -14.925	6.540 5.304	1.00	0.00		3A7
ATOM ATOM	1399	0	LEU	216		-14.143	5.980	1.00	0.00		3A7
ATOM	1391	N	ASP	217		-14.501	4.392	1.00	0.00		3A7
ATOM	1392	CA	ASP	217	24.872	-13.102	4.192	1.00	0.00		3A7
ATOM	1393	CB	ASP	217		-12.608	5.013	1.00	0.00		3A7
ATOM	1394	CG	ASP	217		-13.427	4.786	1.00	0.00		3A7 3A7
ATOM ATOM	1395 1396		ASP ASP	217 217		-12.833 -14.641	4.285 5.118	1.00	0.00		3A7
W T OW	1370	JU2	HOF	211	2		3.110				

ATOM	1397	С	ASP	217	25.056 -	-12.846	2.709	1.00	0.00		3A7
ATOM	1398	ō	ASP	217	26.126		2.166	1.00	0.00		3A7
ATOM	1399	N	PRO	218	24.053 -		2.013	1.00	0.00		3A7
MOTA	1400	CA	PRO	218	24.193 -	-11.689	0.691	1.00	0.00		3A7
ATOM	1401	CD	PRO	218	22.655 -		2.382	1.00	0.00		3A7
MOTA	1402	CB	PRO	218	22.746 ·		0.203	1.00	0.00		3A7
MOTA	1403	CG	PRO	218	21.908		1.050	1.00	0.00		3A7 3A7
MOTA	1404	C	PRO	218	24.945	-10.372 -9.730	0.782 1.833	1.00	0.00		3A7
ATOM	1405	0	PRO	218 219	24.911 25.621	-9.950	-0.316	1.00	0.00		3A7
ATOM	1406 1407	N CA	PHE	219	26.432	-8.745	-0.344	1.00	0.00		3A7
ATOM ATOM	1408	CB	PHE	219	27.591	-8.800	-1.373	1.00	0.00		3A7
ATOM	1409	CG	PHE	219	28.495	-9.952	-1.047	1.00	0.00		3A7
ATOM	1410		PHE	219	29.296	-9.917	0.094	1.00	0.00		3A7
ATOM	1411		PHE	219	28.551	-11.070	-1.881	1.00	0.00		3A7
MOTA	1412	CE1	PHE	219	30.140		0.400	1.00	0.00		3A7
ATOM	1413	CE2	PHE	219	29.393		-1.578	1.00	0.00		3A7
ATOM	1414	CZ	PHE	219	30.189		-0.437	1.00	0.00		3A7
ATOM	1415	С	PHE	219	25.587	-7.501	-0.570	1.00	0.00		3A7 3A7
ATOM	1416	0	PHE	219	25.626	-6.607 -7.366	0.273 -1.669	1.00	0.00		3A7
ATOM	1417	N	VAL	220 220	24.790 24.617	-8.245	-2.807	1.00	0.00		3A7
ATOM ATOM	1418 1419	CA CB	VAL VAL	220	23.148	-8.591	-3.051	1.00	0.00		3A7
ATOM	1420		VAL	220	22.271	-7.323	-3.127	1.00	0.00		3A7
ATOM	1421		VAL	220	22.991	-9.517	-4.277	1.00	0.00		3A7
ATOM	1422	C	VAL	220	25.287	-7.570	-3.983	1.00	0.00		3A7
ATOM	1423	0	VAL	220	25.799	-8.235	-4.883	1.00	0.00		3A7
ATOM	1424	N	LEU	221	25.336	-6.211	-3.963	1.00	0.00		3A7
ATOM	1425	CA	LEU	221	26.163	-5.403	-4.835	1.00	0.00		3A7
MOTA	1426	СВ	LEU	221	25.390	-4.284	-5.597	1.00	0.00		3A7
ATOM	1427	CG	LEU	221	24.479	-4.750	-6.764	1.00	0.00		3A7 3A7
ATOM	1428		LEU	221	25.258	-5.539	-7.835	1.00	0.00		3A7
ATOM	1429		LEU	221	23.213 27.196	-5.501 -4.792	-6.317 -3.913	1.00	0.00		3A7
MOTA	1430	С 0	LEU LEU	221 221	27.196	-5.391	-2.904	1.00	0.00		3A7
ATOM ATOM	1431 1432	N	SER	222	27.682	-3.567	-4.239	1.00	0.00		3A7
ATOM	1433	CA	SER	222	28.622	-2.816	-3.435	1.00	0.00		3A7
ATOM	1434	СВ	SER	222	29.722	-2.139	-4.284	1.00	0.00		3A7
ATOM	1435	ŌĞ	SER	222	30.472	-3.121	-4.985	1.00	0.00		3A7
MOTA	1436	С	SER	222	27.841	-1.762	-2.698	1.00	0.00		3A7
MOTA	1437	0	SER	222	27.764	-0.612	-3.127	1.00	0.00		3A7
MOTA	1438	N	ILE	223	27.222	-2.164	-1.561	1.00	0.00		3A7
MOTA	1439	CA	ILE	223	26.322	-1.338	-0.788	1.00	0.00		3A7 3A7
MOTA	1440	CB	ILE	223	24.971	-2.017	-0.555 -0.110	1.00	0.00		3A7
ATOM	1441		ILE	223 223	25.156 24.042	-3.487 -1.193	0.374	1.00	0.00		3A7
ATOM ATOM	1442 1443	CD	ILE	223	22.603	-1.718	0.416	1.00	0.00		3A7
ATOM	1444	c	ILE	223	27.019	-0.926	0.488	1.00	0.00	•	3A7
ATOM	1445	ŏ	ILE	223	27.093	0.266	0.787	1.00	0.00		3A7
ATOM	1446	N	LYS	224	27.556	-1.893	1.271	1.00	0.00		3A7
MOTA	1447	CA	LYS	224	28.263	-1.581	2.490	1.00	0.00		3A7
ATOM	1448	СВ	LYS	224	27.339	-1.185	3.674	1.00	0.00		3A7
ATOM	1449	CG	LYS	224	28.088	-0.528	4.849	1.00	0.00		3A7
MOTA	1450	CD	LYS	224	27.190	-0.187 -1.411	6.049 6.861	1.00	0.00		3A7 3A7
MOTA	1451	CE	LYS	224	26.740	-2.112	7.458	1.00	0.00		3A7
MOTA MOTA	1452 1453	NZ	LYS LYS	224 224	27.901 29.052	-2.796	2.890	1.00	0.00		3A7
ATOM	1454	С 0	LYS	224	30.070	-2.683	3.572	1.00	0.00		3A7
ATOM	1455	N	VAL	225	28.582	-4.008	2.483	1.00	0.00		3A7
ATOM	1456	CA	VAL	225	29.124	-5.288	2.907	1.00	0.00		3A7
MOTA	1457	СВ	VAL	225	28.125	-6.430	2.746	1.00	0.00		3A7
ATOM	1458		VAL	225	28.683	-7.731	3.365	1.00	0.00		3A7
ATOM	1459		VAL	225	26.805	-6.017	3.429	1.00	0.00		3A7
MOTA	1460	С	VAL	225	30.398	-5.583	2.147	1.00	0.00		3A7
MOTA	1461	0	VAL	225	31.486	-5.449	2.708	1.00	0.00		3A7 3A7
ATOM	1462	N	PHE	226	30.271	-5.986	0.851 -0.106	1.00	0.00		3A7
ATOM	1463	CA CB	PHE	226 226	31.349 32.367	-6.182 -4.997	-0.108	1.00	0.00		3A7
MOTA MOTA	1464 1465	CG	PHE	226	33.203	-4.921	-1.346	1.00	0.00		3A7
ATOM	1466		PHE	226	34.585	-5.107	-1.283	1.00	0.00		3A7
ATOM	1467		PHE	226	32.615	-4.631	-2.578	1.00	0.00		3A7
ATOM	1468		PHE	226	35.365	-5.025	-2.432	1.00	0.00		3A7

ATOM	1469	CE2	PHE	226	33.393	-4.550	-3.730	1.00	0.00	3A7
	1470	cz	PHE	226	34.768	-4.749	-3.658	1.00	0.00	3A7
MOTA						-7.514	0.144	1.00	0.00	3A7
ATOM	1471	С	PHE	226	32.059					
ATOM	1472	0	PHE	226	32.151	-7.943	1.295	1.00	0.00	3A7
ATOM	1473	N	PRO	227	32.610	-8.198	-0.871	1.00	0.00	3A7
	1474	CA	PRO	227	33.431	-9.392	-0.698	1.00	0.00	3A7
MOTA						-8.089	-2.237	1.00	0.00	3A7
MOTA	1475	CD	PRO	227	32.111					
ATOM	1476	ÇВ	PRO	227	33.602	-9.944	-2.123	1.00	0.00	3A7
MOTA	1477	CG	PRO	227	32.349	-9.465	-2.857	1.00	0.00	3A7
			PRO	227	34.778	-9.081	-0.061	1.00	0.00	3A7
ATOM	1478	C					0.062	1.00	0.00	3A7
MOTA	1479	0	PRO	227	35.140	-7.911				
ATOM	1480	N	PHE	228	35.535	-10.132	0.346	1.00	0.00	3A7
ATOM	1481	CA	PHE	228	36.792	-10.004	1.060	1.00	0.00	3A7
		СВ	PHE	228	37.130	-11.255	1.926	1.00	0.00	3A7
MOTA	1482				37.053		1.172	1.00	0.00	3A7
ATOM	1483	CG	PHE	228						3A7
ATOM	1484	CD1	PHE	228	35.821		0.937	1.00	0.00	
ATOM	1485	CD2	PHE	228	38.217	-13.193	0.733	1.00	0.00	3A7
ATOM	1486	CEL		228	35.753	-14.388	0.257	1.00	0.00	3A7
					38.152		0.053	1.00	0.00	3A7
MOTA	1487		PHE	228					0.00	3A7
ATOM	1488	CZ	PHE	228	36.919		-0.187	1.00		
ATOM	1489	С	PHE	228	37.924	-9.676	0.107	1.00	0.00	3A7
ATOM	1490	o	PHE	228	38.323	-10.488	-0.727	1.00	0.00	3A7
					38.440	-8.432	0.225	1.00	0.00	3A7
ATOM	1491	N	LEU	229					0.00	3A7
MOTA	1492	CA	LEU	229	39.469	-7.914	-0.636	1.00		
ATOM	1493	CB	LEU	229	38.924	-7.440	-2.010	1.00	0.00	3A7
ATOM	1494	CG	LEU	229	39.979	-6.871	-2.990	1.00	0.00	3A7
				229	41.083	-7.892	-3.326	1.00	0.00	3A7
ATOM	1495		LEU					1.00	0.00	3A7
ATOM	1496	CD2	LEU	229	39.305	-6.347	-4.273			
ATOM	1497	C	LEU	229	40.062	-6.752	0.105	1.00	0.00	3A7
ATOM	1498	0	LEU	229	41.281	-6.639	0.226	1.00	0.00	3A7
ATOM	1499	N	THR	230	39.186	-5.847	0.615	1.00	0.00	3A7
					39.568	-4.636	1.308	1.00	0.00	3A7
ATOM	1500	CA	THR	230						3A7
ATOM	1501	CB	THR	230	38.715	-3.444	0.870	1.00	0.00	
MOTA	1502	OG1	THR	230	39.184	-2.215	1.417	1.00	0.00	3A7
ATOM	1503	CG2	THR	230	37.220	-3.639	1.206	1.00	0.00	3A7
	1504	c	THR	230	39.476	-4.902	2.807	1.00	0.00	3A7
ATOM						-5.527	3.250	1.00	0.00	3A7
ATOM	1505	0	THR	230	38.513					3A7
ATOM	1506	N	PRO	231	40.435	-4.450	3.626	1.00	0.00	
ATOM	1507	CA	PRO	231	40.382	-4.534	5.074	1.00	0.00	3A7
ATOM	1508	CD	PRO	231	41.737	-3.996	3.151	1.00	0.00	3A7
				231	41.866	-4.556	5.472	1.00	0.00	3A7
ATOM -	1509	CB	PRO						0.00	3A7
ATOM	1510	CG	PRO	231	42.555	-3.696	4.409	1.00		
MOTA	1511	С	PRO	231	39.661	-3.313	5.625	1.00	0.00	3A7
ATOM .	1512	0	PRO	231	38.946	-2.637	4.885	1.00	0.00	3A7
	1513	N	ILE	232	39.877	-3.024	6.939	1.00	0.00	3A7
ATOM							7.738	1.00	0.00	3A7
ATOM	1514	CA	ILE	232	39.462	-1.870				
ATOM	1515	CB	ILE	232	40.410	-0.663	7.563	1.00	0.00	3A7
ATOM	1516	CG2	ILE	232	40.450	-0.093	6.123	1.00	0.00	3A7
ATOM	1517		ILE		40.186	0.463	8,608	1.00	0.00	3A7
						0.068	10.038	1.00	0.00	3A7
ATOM	1518	CD	ILE	232	40.563				0.00	3A7
ATOM	1519	С	ILE	232	37.983	-1.493	7.610	1.00		
ATOM	1520	0	ILE	232	37.631	-0.517	6.949	1.00	0.00	3A7
ATOM	1521	N	LEU	233	37.047	-2.244	8.259	1.00	0.00	3A7
ATOM	1522	CA	LEU	233	37.231	-3.488	8.977	1.00	0.00	3A7
					36.638	-3.490	10.418	1.00	0.00	3A7
MOTA	1523	CB	LEU	233						3A7
MOTA	1524	CG	LEU	233	37.361	-2.613	11.475	1.00	0.00	
ATOM	1525	CD1	LEU	233	38.832	-3.029	11.668	1.00	0.00	3A7
ATOM	1526	CD2	LEU	233	37.198	-1.098	11.249	1.00	0.00	3A7
ATOM	1527	c	LEU	233	36.518	-4.523	8.138	1.00	0.00	3A7
								1.00	0.00	3A7
ATOM	1528	0	LEU	233	36.754	-4.608	6.933			
ATOM	1529	N	GLU	234	35.621	-5.330	8.775	1.00	0.00	3A7
ATOM	1530	CA	GLU	234	34.755	-6.337	8.183	1.00	0.00	3A7
ATOM	1531	CB	GLU	234	33.985	-5.836	6.925	1.00	0.00	3A7
					32.750	-6.666	6.514	1.00	0.00	3A7
ATOM	1532	CG	GLU	234				1.00	0.00	3A7
ATOM	1533	CD	GLU	234	33.141	-7.946	5.777			
MOTA	1534	OE1	GLU	234	33.797	-7.837	4.707	1.00	0.00	3A7
ATOM	1535		GLU	234	32.780	-9.048	6.271	1.00	0.00	3A7
			GLU	234	35.545	-7.587	7.877	1.00	0.00	3A7
MOTA	1536	C						1.00	0.00	3A7
ATOM	1537	0	GLU	234	36.385	-7.576	6.978			
MOTA	1538	N	ALA	. 235	35.267	-8.681	8.642	1.00	0.00	3A7
ATOM	1539	CA	ALA	235	35.833	-10.014	8.499	1.00	0.00	3A7
	1540	СВ	ALA	235		-10.390	7.067	1.00	0.00	3A7
MOTA	1340	CB	TUT		54.205					

ATOM	1541	С	ALA	235	37.017	-10.214	9.409	1.00	0.00	3A7
ATOM	1542	0	ALA	235		-11.312	9.899	1.00	0.00	3A7
ATOM	1543	N	LEU	236	37.790	-9.141	9.671	1.00	0.00	3A7
ATOM	1544	CA	LEU	236	38.971	-9.206	10.503	1.00	0.00	3A7 3A7
MOTA	1545	CB	LEU	236	39.828	-7.935	10.361 8.906	1.00	0.00 0.00	3A7
MOTA	1546	CG	LEU	236 236	40.242 40.964	-7.612 -6.254	8.836	1.00	0.00	3A7
ATOM	1547		LEU	236	41.094	-8.728	8.272	1.00	0.00	3A7
MOTA MOTA	1548 1549	C	LEU	236	38.601	-9.366	11.956	1.00	0.00	3A7
ATOM	1550	Ö	LEU	236		-10.138	12.697	1.00	0.00	3A7
ATOM	1551	N	ASN	237	37.530	-8.664	12.387	1.00	0.00	3A7
ATOM	1552	CA	ASN	237	37.020	-8.738	13.741	1.00	0.00	3A7
ATOM	1553	СВ	ASN	237	35.917	-7.685	13.982	1.00	0.00	3A7
MOTA	1554	CG	ASN	237	36.463	-6.273	13.746	1.00	0.00	3A7
ATOM	1555		ASN	237	35.922	-5.526	12.923	1.00	0.00	3A7
ATOM	1556		ASN	237	37.544	-5.910	14.500	1.00	0.00	3A7 3A7
ATOM	1557	C	ASN	237		-10.107	14.022 15.111	1.00	0.00	3A7
ATOM	1558	0	ASN	237 238		-10.658 -10.707	12.979	1.00	0.00	3A7
ATOM ATOM	1559 1560	N CA	ILE	238		-12.011	13.021	1.00	0.00	3A7
ATOM	1561	CB	ILE	238		-12.290	11.743	1.00	0.00	3A7
ATOM	1562		ILE	238		-13.648	11.845	1.00	0.00	3A7
ATOM	1563		ILE	238		-11.141	11.432	1.00	0.00	3A7
ATOM	1564	CD	ILE	238	32.367	-10.932	12.495	1.00	0.00	3A7
ATOM	1565	С	ILE	238	36.280	-13.064	13.260	1.00	0.00	3A7
ATOM	1566	٥	ILE	238		-13.896	14.106	1.00	0.00	3A7
ATOM	1567	N	THR	239		-13.013	12.556	1.00	0.00	3A7
ATOM	1568	CA	THR	239		-13.929	12.699	1.00	0.00 0.00	3A7 3A7
ATOM	1569	CB	THR	239		-13.767 -13.766	11.574 10.323	1.00	0.00	3A7
ATOM ATOM	1570 1571		THR THR	239 239		-14.928	11.571	1.00	0.00	3A7
ATOM	1572	C	THR	239		-13.773	14.033	1.00	0.00	3A7
ATOM	1573	ŏ	THR	239		-14.740	14.603	1.00	0.00	3A7
ATOM	1574		VAL	240		-12.555	14.619	1.00	0.00	3A7
ATOM	1575	CA	VAL	240	39.759	-12.276	15.932	1.00	0.00	3A7
ATOM	1576	CB	VAL	240		-10.784	16.162	1.00	0.00	3A7
ATOM	1577		VAL	240		-10.421	17.627	1.00	0.00	3A7
ATOM	1578		VAL	240		-10.316	15.239	1.00	0.00	3A7 3A7
MOTA	1579	C	VAL	240		-12.842 -13.460	17.025 17.956	1.00	0.00	3A7
MOTA MOTA	1580 1581	0	VAL PHE	240 241		-12.667	16.920	1.00	0.00	3A7
ATOM	1582	N CA	PHE	241		-13.266	17.837	1.00	0.00	. 3A7
ATOM	1583	.CB	PHE	241		-12.893	17.483	1.00	0.00	3A7
ATOM	1584	CG	PHE	241		-14.041	17.098	1.00	0.00	. 3A7
MOTA	1585	CD1	PHE	241		-15.104	17.973	1.00	0.00	3A7
ATOM	1586		PHE	241		-14.250	15.746	1.00	0.00	3A7
ATOM	1587		PHE	241		-16.400	17.483	1.00	0.00	3A7
ATOM	1588		PHE	241		-15.545	15.244	1.00	0.00	3A7 3A7
ATOM	1589	ÇZ	PHE	241		-16.626 -14.763	16.119 17.938	1.00	0.00	3A7
ATOM ATOM	1590 1591	0	PHE	241 241		-15.276	19.050	1.00	0.00	3A7
ATOM	1592	N	PRO	242		-15.511	16.814	1.00	0.00	3A7
ATOM	1593	CA	PRO	242		-16.902	16.784	1.00	0.00	3A7
ATOM	1594	CD	PRO	242		~15.196	15.686	1.00	0.00	3A7
ATOM	1595	CB	PRO	242	36.945	-17.375	15.333	1.00	0.00	3A7
MOTA	1596	CG	PRO	242		-16.221	14.553	1.00	0.00	3A7
ATOM	1597	С	PRO	242		-17.310	17.435	1.00	0.00	3A7
ATOM	1598	0	PRO	242		-18.268	18.191	1.00	0.00	3A7 3A7
ATOM	1599	N	ARG	243		-16.603	17.262 17.893	1.00	0.00	3A7
MOTA MOTA	1600 1601	CA CB	ARG ARG	243 243		-16.892 -15.942	17.355	1.00	0.00	3A7
ATOM	1601	CG	ARG	243		-16.265	15.917	1.00	0.00	3A7
ATOM	1603	CD	ARG	243		-15.187	15.348	1.00	0.00	3A7
ATOM	1604	NE	ARG	243		-15.532	13.927	1.00	0.00	3A7
ATOM	1605	CZ	ARG	243	44.062	-14.651	13.096	1.00	0.00	3A7
ATOM	1606		ARG	243		-15.003	11.800	1.00	0.00	3A7
ATOM	1607		ARG	243		-13.422	13.549	1.00	0.00	3A7
MOTA	1608	C	ARG	243		-16.769	19.398	1.00	0.00	3A7 3A7
ATOM	1609	0	ARG	243		-17.580 -15.774	20.122 19.905	1.00	0.00	3A7
ATOM	1610 1611	N CA	LYS LYS	244 244		-15.774	21.327	1.00	0.00	3A7
MOTA MOTA	1612	CB	LYS	244		-14.178	21.648	1.00	0.00	3A7

ATOM	1613	CG	LYS	244	39.241	-13.772	23.119	1.00	0.00	3A7
MOTA	1614	CD	LYS	244	39.058		23.402		0.00	3A7
MOTA	1615	CE	LYS	244	40.110		22.745	1.00	0.00	3A7 3A7
ATOM	1616	NZ	LYS	244	41.474 · 38.844 ·		23.205	1.00	0.00	3A7
ATOM ATOM	1617 1618	С О	LYS	244 244	39.175		23.051	1.00	0.00	3A7
ATOM	1619	N	VAL	245	37.806		21.259	1.00	0.00	3A7
ATOM	1620	CA	VAL	245	37.014		21.692	1.00	0.00	3A7
ATOM	i621	СВ	VAL	245	35.821	-18.595	20.774	1.00	0.00	3A7
ATOM	1622		VAL	245	35.055		21.138	1.00	0.00	3A7
MOTA	1623		VAL	245	34.893 37.868		20.861 21.753	1.00	0.00 0.00	3A7 3A7
ATOM	1624 1625	C 0	VAL VAL	245 245	37.867		22.748	1.00	0.00	3A7
ATOM ATOM	1626	N	ILE	246	38.674		20.690	1.00	0.00	3A7
ATOM	1627	CA	ILE	246	39.563		20.600	1.00	0.00	3A7
ATOM	1628	СB	ILE	246	40.252		19.232	1.00	0.00	3A7
ATOM	1629		ILE	246	41.696		19.259	1.00	0.00	3A7
MOTA	1630		ILE	246	39.414 38.083		18.224 17.793	1.00	0.00	3A7 3A7
ATOM ATOM	1631 1632	CD	ILE	246 246	40.571		21.724	1.00	0.00	3A7
ATOM	1633	Ö	ILE	246	40.828		22.332	1.00	0.00	3A7
MOTA	1634	N	SER	247	41.133		22.059	1.00	0.00	3A7
ATOM	1635	CA	SER	247	42.119	-19.652	23.098	1.00	0.00	3A7
MOTA	1636	СВ	SER	247	42.734		23.119	1.00	0.00	3A7
ATOM	1637	oG	SER	247	43.425 41.551		21.903 24.461	1.00	0.00	3A7 3A7
ATOM ATOM	1638 1639	C O	SER SER	247 247	42.194		25.271	1.00	0.00	3A7
ATOM	1640	N	PHE	248	40.320		24.749	1.00	0.00	3A7
ATOM	1641	CA	PHE	248	39.670		26.022	1.00	0.00	3A7
ATOM	1642	СВ	PHE	248	38.328		26.125	1.00	0.00	3A7
ATOM	1643	CG	PHE	248	38.514		26.559	1.00	0.00	3A7 . 3A7
ATOM	1644		PHE	248	37.951 39.191		25.828 27.745	1.00	0.00	. 3A7
ATOM ATOM	1645 1646		PHE	248 248	38.058		26.274	1.00	0.00	3A7
ATOM	1647		PHE	248	39.316		28.183	1.00	0.00	3A7
ATOM	1648	CZ	PHE	248	38.749		27.447	1.00	0.00	3A7
ATOM	1649	С	PHE	248	39.389		26.244	1.00	0.00	3A7
MOTA	1650	0	PHE	248	39.623		27.323	1.00	0.00	3A7 3A7
ATOM ATOM	1651 1652	N CA	LEU	249 249	38.919 38.585		25.198 25.317	1.00	0.00	3A7
ATOM	1653	СВ	LEU	249		-23.699	24.147	1.00	0.00	3A7
ATOM	1654	CG	LEU	249	36.376	-22.962	24.103	1.00	0.00	3A7
ATOM	1655		LEU	249		-23.308	22.821	1.00	0.00	3A7
MOTA	1656		LEU	249		-23.243	25.342	1.00	0.00	3A7 3A7
ATOM	1657	С 0	LEU.	249 _. 249		-24.111 -25.088	25.396 26.140	1.00	0.00	3A7
ATOM .	1658 1659	N	THR	250		-23.744	24.670	1.00	0.00	3A7
ATOM	1660	CA	THR	250	42.150		24.706	1.00	0.00	3A7
ATOM .	1661	CB	THR	250	43.131	-23.926	23.673	1.00	0.00	3A7
MOTA	1662		THR	250		-24.120	22.372	1.00	0.00	3A7
ATOM	1663		THR	250		-24.649	23.731 26.085	1.00	0.00	3A7 3A7
MOTA MOTA	1664 1665	С 0	THR THR	250 250		-24.398 -25.376	26.573	1.00	0.00	3A7
ATOM	1666	N	LYS	251		-23.243	26.777	1.00	0.00	3A7
ATOM	1667	CA	LYS	251		-23.060	28.132	1.00	0.00	3A <u>7</u>
MOTA	1668	СВ	LYS	251		-21.601	28.592	1.00	0.00	3A7
ATOM	1669	CG	LYS	251		-21.282	29.945	1.00	0.00	3A7
ATOM	1670	CD	LYS	251 251		-19.803 -19.494	30.335 31.700	1.00	0.00	3A7 3A7
ATOM ATOM	1671 1672	CE NZ	LYS LYS	251		-18.062	32.038	1.00	0.00	3A7
ATOM	1673	c	LYS	251		-23.933	29.091	1.00	0.00	3A7
ATOM	1674	ō	LYS	251	42.946	-24.559	29.945	1.00	0.00	3A7
MOTA	1675	N	SER	252		-24.057	28.942	1.00	0.00	3A7
MOTA	1676	CA	SER	252		-24.912	29.776	1.00	0.00	3A7 3A7
ATOM	1677	CB	SER	252 252		-24.780 -23.431	29.422 29.562	1.00	0.00	3A7
MOTA MOTA	1678 1679	OG C	SER SER	252 252		-25.431	29.662	1.00	0.00	3A7
ATOM	1680	ŏ	SER	252		-27.089	30.653	1.00	0.00	3A7
MOTA	1681	N	VAL	253	40.836	-26.832	28.425	1.00	0.00	3A7
MOTA	1682	CA	VAL	253		-28.203	28.125	1.00	0.00	3A7
MOTA	1683	CB	VAL	253		-28.416	26.609	1.00	0.00	3A7 3A7
MOTA	1684	CG1	VAL	253	41.865	-29.803	26.237	1.00	0.00	3A /

	ATOM	1685	CG2	VAL	253	39.886	-28.264	25.997	1.00	0.00	3A7
	ATOM	1686	C	VAL	253	42.532		28.758	1.00	0.00	3A7
	ATOM	1687	0	VAL	253	42.684		29.404	1.00	0.00	3A7
	ATOM	1688	N	LYS	254	43.518		28.616	1.00	0.00	3A7
	ATOM	1689	CA	LYS	254	44.842		29.162	1.00	0.00	3A7
	ATOM	1690	СВ	LYS	254	45.735		28.706	1.00	0.00	3A7
	ATOM	1691	CG	LYS	254	47.220		29.086	1.00	0.00	3A7 3A7
	MOTA	1692	CD	LYS	254	48.143		28.496 29.199	1.00	0.00	3A7
	MOTA	1693	CE	LYS	254	48.079 46.811		28.925	1.00	0.00	3A7
	ATOM	1694 1695	NZ C	LYS LYS	254 254	44.830		30.665	1.00	0.00	3A7
	ATOM ATOM	1696	0	LYS	254	45.412		31.270	1.00	0.00	3A7
	HOTA	1697	N	GLN	255	44.098		31.313	1.00	0.00	3A7
	ATOM	1698	CA	GLN	255 .	43.943		32.753	1.00	0.00	3A7
	ATOM	1699	СВ	GLN	255	43.122	-25.635	33.238	1.00	0.00	3A7
	ATOM	1700	CG	GLN	255	43.863	-24.302	33.045	1.00	0.00	3A7
	ATOM	1701	CD	GLN	255	42.977	-23.153	33.535	1.00	0.00	3A7
	ATOM	1702	OE1	GLN	255		-22.444	34.484	1.00	0.00	3A7
	ATOM	1703	NE2		255	41.801		32.860	1.00	0.00	3A7
	ATOM	1704	С	GLN	255		-28.104	33.282	1.00	0.00	3A7 3A7
	MOTA	1705	0	GLN	255	43.599		34.372	1.00	0.00	3A7
	MOTA	1706	N	ILE	256		-28.710 -29.907	32.490 32.888	1.00	0.00	3A7
	ATOM	1707	CA CB	ILE	256 256		-30.098	32.072	1.00	0.00	3A7
	ATOM ATOM	1708 1709		ILE ILE	256		-31.597	31.831	1.00	0.00	3A7
	ATOM	1710		ILE	256		-29.508	32.862	1.00	0.00	3A7
	MOTA	1711	CD	ILE	256		-28.036	33.277	1.00	0.00	3A7
	ATOM	1712	c	ILE	256		-31.136	32.826	1.00	0.00	3A7
	ATOM	1713	0	ILE	256	42.411	-32.060	33.627	1.00	0.00	3A7
	MOTA	1714	N	LYS	257		-31.169	31.881	1.00	0.00	3A7
	MOTA	1715	CA	LYS	257		-32,272	31.759	1.00	0.00	3A7
	MOTA	1716	CB	LYS	257		-32.240	30.418	1.00	0.00	3A7
	MOTA	1717	CG	LYS	257		-32.548	29.218	1.00	0.00	3A7 3A7
	ATOM	1718	CD	LYS	257		-32.676	27.864 27.283	1.00 1.00	0.00	3A7
	MOTA	1719	CE	LYS	257 257		-31.365 -30.908	27.203	1.00	0.00	3A7
	ATOM	1720 1721	NZ C	LYS LYS	257		-32.284	32.873	1.00	0.00	3A7
	ATOM ATOM	1722	0	LYS	257		-33.343	33.303	1.00	0.00	3A7
	ATOM	1723	N	GLU	258		-31.083	33.378	1.00	0.00	3A7
	ATOM	1724	CA	GLU	258		-30.925	34.446	1.00	0.00	3A7
	ATOM	1725	СВ	GLU	258	47.454	-29.519	34.428	1.00	0.00	3A7
	ATOM	1726	CG	GLU	258	48.242	-29.217	33.141	1.00	0.00	3A7
	ATOM	1727	CD	GLU	258		-30.199	33.003	1.00	0.00	3A7
	MOTA	1728		GLU	258		-30.202	33.900	1.00	0.00	3A7
	ATOM	1729		GLU	258		-30.958	31.997	1.00	0.00	3A7 3A7
	ATOM	1730	С	GLU	258		-31.151	35.797	1.00	0.00	3A7 3A7
	MOTA	1731	0	GLU	258		-31.501 -30.971	36.763 35.870	1.00	0.00	3A7
	MOTA	1732 1733	N CA	GLY GLY	259 259		-31.194	37.052	1.00	0.00	3A7
•	ATOM ATOM	1734		GLY	259		-32.598	37.051	1.00	0.00	3A7
	ATOM	1735	o	GLY	259		-33.461	36.340	1.00	0.00	3A7
	ATOM	1736	N	ARG	260		-32.842	37.887	1.00	0.00	3A7
	ATOM	1737	CA	ARG	260		-34.118	38.133	1.00	0.00	3A7
	ATOM	1738	CB	ARG	260	41.489	-34.954		1.00	0.00	3A7
	MOTA	1739	CG	ARG	260		-36.233	37.027	1.00	0.00	3A7
	MOTA	1740	CD	ARG	260		-36.004	37.425	1.00	0.00	3A7
	MOTA	1741	NE	ARG	260		-35.667	38.882	1.00	0.00	3A7 3A7
	ATOM	1742	CZ	ARG	260		-35.260	39.486	1.00	0.00	3A7
	ATOM	1743		ARG	260 260		-34.927 -35.174	40.809 38.781	1.00	0.00	3A7
	MOTA MOTA	1744 1745	C	ARG ARG	260		-34.898	39.116	1.00	0.00	3A7
	ATOM	1746	ō	ARG	260		-35.831	38.749	1.00	0.00	3A7
	ATOM	1747	N	LEU	261		-34.475	40.403	1.00	0.00	3A7
	ATOM	1748	CA	LEU	261		-34.943	41.438	1.00	0.00	3A7
	ATOM	1749	СВ	LEU	261		-33.853	41.945	1.00	0.00	3A7
	ATOM	1750	CG	LEU	261		-32.584	42.630	1.00	0.00	3A7
	ATOM	1751		LEU	261		-31.737	43.230	1.00	0.00	3A7
	MOTA	1752		LEU	261		-31.708	41.709	1.00	0.00	3A7
	ATOM	1753	С	LEU	261		-35.510	42.582	1.00	0.00	3A7 3A7
	ATOM	1754	0	LEU	261		-36.544	43.138	1.00	0.00	3A7 3A7
	ATOM	1755	N	LYS	262 262		-34.835 -35.239	42.973 44.117	1.00	0.00	3A7
	MOTA	1756	CA	LYS	402	30.700	33.233	77.11/	1.00		

ATOM	1757	СВ	LYS	262	41.421 -	34.790	45.462	1.00	0.00	3A7
ATOM	1758	CG	LYS	262	40.810 -		46.708	1.00	0.00	3A7
ATOM	1759	CD	LYS	262	41.515 -		48.009	1.00	0.00	3A7
ATOM	1760	CE	LYS	262	41.066 -		49.233	1.00	0.00	3A7 3A7
ATOM	1761	NZ	LYS	262	39.611 -		49.468	1.00	0.00	3A7
ATOM	1762	C	LYS	262	39.442 - 39.325 -		43.941 43.313	1.00	0.00	3A7
ATOM	1763	0	LYS GLU	262 263	38.381 -		44.510	1.00	0.00	3A7
ATOM ATOM	1764 1765	N CA	GLU	263	37.009 -		44.438	1.00	0.00	3A7
ATOM	1766	CB	GLU	263	36.001		44.396	1.00	0.00	3A7
ATOM	1767	CG	GLU	263	36.178 -		43.152	1.00	0.00	3A7
ATOM	1768	CD	GLU	263	35.147 -	-37.964	43.149	1.00	0.00	3A7
MOTA	1769	OE1	GLU	263	34.322		44.098	1.00	0.00	3A7
ATOM	1770		GLU	263	35.174 -		42.183	1.00	0.00	3A7 3A7
MOTA	1771	С	GLU	263	36.698		45.630 46.501	1.00	0.00	3A7
ATOH	1772	0	GLU	263	35.910 · 37.333 ·		45.670	1.00	0.00	3A7
ATOM	1773 1774	N CA	THR THR	264 264	37.170		46.715	1.00	0.00	3A7
ATOM ATOM	1775	CB	THR	264	38.280		47.757	1.00	0.00	3A7
ATOM	1776		THR	264	38.329		48.352	1.00	0.00	3A7
ATOM	1777		THR	264	38.047	-30.721	48.870	1.00	0.00	3A7
ATOM	1778	С	THR	264	37.164	-30.395	46.003	1.00	0.00	3A7
MOTA	1779	0	THR	264	36.480		46.415	1.00	0.00	3A7
MOTA	1780	N	GLN	265	37.940		44.890	1.00	0.00	3A7 3A7
ATOM	1781	CA	GLN	265	38.063		44.052 43.298	1.00	0.00	3A7
ATOM	1782	CB	GLN	265 265	39.417 · 40.645 ·		44.201	1.00	0.00	3A7
ATOM ATOM	1783 1784	CG CD	GLN GLN	265	40.965		45.032	1.00	0.00	3A7
ATOM	1785		GLN	265	41.070		44.497	1.00	0.00	3A7
ATOM	1786		GLN	265	41.132		46.374	1.00	0.00	3A7
ATOM	1787	С	GLN	265	36.953	-29.140	43.030	1.00	0.00	3A7
ATOM	1788	0	GLN	265	36.287		42.802	1.00	0.00	3A7
MOTA	1789	N	LYS	266	36.738		42.404	1.00	0.00	3A7 3A7
MOTA	1790	CA	LYS	266	35.642		41.500	1.00	0.00	3A7
ATOM	1791	CB	LYS	266	36.035 · 37.305 ·		40.002 39.591	1.00	0.00	3A7
ATOM ATOM	1792 1793	CG CD	LYS LYS	266 266	37.703		38.129	1.00	0.00	3A7
ATOM	1794	CE	LYS	266	38.982		37.724	1.00	0.00	3A7
ATOM	1795	NZ	LYS	266	39.346		36.320	1.00	0.00	3A7
ATOM	1796	C	LYS	266	35.129	-31.922	41.858	1.00	0.00	3A7
MOTA	1797	0	TA2		35.796		41.655	1.00	0.00	3A7
MOTA	1798	N	HIS	267	33.902		42.437	1.00	0.00	3A7 3A7
ATOM	1799	CA	HIS	267	33.272		42.940 45.499	1.00	0.00	3A7
ATOM	1800 1801	CC	HIS HIS	267 267	32.504	-34.098		1.00	0.00	3A7
ATOM ATOM	1802	СВ	HIS	267	32.380		44.174	1.00	0.00	3A7
ATOM	1803		HIS	267	30.385		45.524	1.00	0.00	3A7
ATOM	1804	CD2	HIS	267	. 30.489	-34.526	44.840	1.00	0.00	3A7
MOTA	1805	CEI	HIS		31.620		45,901	1.00	0.00	3A7
ATOM	1806	С	HIS	267	32.435		41.858	1.00	0.00	3A7 3A7
MOTA	1807	0	HIS	267	32.255 31.909		41.834	1.00	0.00	3A7
ATOM ATOM	1808 1809	N CA	ARG ARG	268 268	31.110		39.804	1.00	0.00	3A7
ATOM	1810	CB	ARG	268	29.939		39.501	1.00	0.00	3A7
ATOM	1811	CG	ARG	268	30.357		39.172	1.00	0.00	3A7
ATOM	1812	CD	ARG	268	29.154		38.948	1.00	0.00	3A7
ATOM	1813	NE	ARG	268	29.664		38.573	1.00	0.00	3A7
MOTA	1814	CZ	ARG	268	28.818		38.353	1.00	0.00	3A7
MOTA	1815		ARG	268	29.328		37.993	1.00	0.00	3A7 3A7
ATOM	1816		ARG	268	27.470 31.997		38.491 38.593	1.00	0.00	3A7
ATOM	1817	C O	ARG ARG	268 268	33.012		38.485	1.00	0.00	3A7
ATOM ATOM	1818 1819	И	VAL	269	31.604		37.643	1.00	0.00	3A7
ATOM	1820	CA	VAL	269	32.279		36.378	1.00	0.00	3A7
ATOM	1821	СВ	VAL	269	32.595	-36.021	36.063	1.00	0.00	3A7
ATOM	1822		VAL	269	33.733		37.001	1.00	0.00	3A7
MOTA	1823		VAL	269	31.340		36.220	1.00	0.00	3A7 3A7
ATOM	1824	C	VAL	269		-33.947	35.315	1.00	0.00	3A7
ATOM	1825	0	VAL	269 270		-33.712 -33.642	35.519 34.156	1.00	0.00	3A7
ATOM ATOM	1826 1827	N CA	ASP ASP	270	31.450		33.096	1.00	0.00	3A7
ATOM	1828	CB	ASP	270		-31.399	33.132	1.00	0.00	3A7

ATOM	1829	CG	ASP	270	33.510 -	31.368	33.034	1.00	0.00	3A7
MOTA	1830	OD1		270	34.013 -		31.995	1.00	0.00	3A7 3A7
ATOM	1831		ASP	270	34.191 -		33.998 31.781	1.00	0.00	3A7
MOTA MOTA	1832 1833	С 0	ASP ASP	270 270	31.710 - 32.369 -		31.709	1.00	0.00	3A7
ATOM	1834	N	PHE	271	31.187 -		30.684	1.00	0.00	3A7
ATOM	1835	CA	PHE	271	31.302 -		29.357	1.00	0.00	3A7
MOTA	1836	CB	PHE	271	30.407 -		28.356 27.080	1.00	0.00 0.00	3A7 3A7
ATOM ATOM	1837 1838	CG	PHE	271 271	30.344 - 30.012 -		27.101	1.00	0.00	3A7
ATOM	1839		PHE	271	30.758 -		25.887	1.00	0.00	3A7
ATOM	1840		PHE	271	30.211 -		25.972	1.00	0.00	3A7
ATOM	1841		PHE	271	30.870 - 30.646 -		24.737 24.793	1.00	0.00	3A7 3A7
MOTA ATOM	1842 1843	CZ C	PHE	271 271	32.719 -		28.848	1.00	0.00	3A7
ATOM	1844	ŏ	PHE	271	33.150 -		28.204	1.00	0.00	3A7
MOTA	1845	N	LEU	272	33.494 -		29.146	1.00	0.00	3A7
ATOM	1846	CA	LEU	272	34.866 -		28.716	1.00	0.00 0.00	3A7 3A7
ATOM ATOM	1847 1848	CB CG	LEU	272 272	35.455 - 36.816 -		29.100 28.482	1.00	0.00	3A7
	1849		LEU	272	36.864 -		28.078	1.00	0.00	3A7
ATOM	1850		LEU	272	38.027 -	-31.011	29.363	1.00	0.00	3A7
ATOM	1851	С	LEU	272	35.735 -		29.311	1.00	0.00	3A7 3A7
ATOM	1852 1853	O N	LEU	272 273	36.573 - 35.522 -		28.634 30.606	1.00	0.00	3A7
ATOM ATOM	1854	CA	GLN	273	36.255 -		31.288	1.00	0.00	3A7
ATOM	1855	СВ	GLN	273	35.890 -		32.788	1.00	0.00	3A7
ATOM	1856	CG	GLN	273	36.853 -		33.658	1.00	0.00	3A7 3A7
ATOM	1857 1858	CD	GLN GLN	273 273	38.222 - 38.361 -		33.686 34.234	1.00	0.00	3A7
ATOM ATOM	1859		GLN	273	39.247 -		33.079	1.00	0.00	3A7
ATOM	1860	С	GLN	273	35.971 -		30.668	1.00	0.00	3A7
ATOM	1861	0	GLN	273	36.882 -		30.456	1.00	0.00	3A7 3A7
ATOM .	1862 1863	N CA	LEU	274 274	34.685 - 34.245 -		30.310 29.669	1.00	0.00	3A7
ATOM	1864	CB	LEU	274	32.718 -		29.471	1.00	0.00	3A7
ATOM	1865	CG	LEU	274	31.891 -		30.761	1.00	0.00	3A7
ATOM	1866		LEU	274	30.398		30.394	1.00	0.00	3A7 3A7
ATOM ATOM	1867 1868	CD2	LEU	274 274	32.273 · 34.854 ·		31.558 28.302	1.00	0.00	3A7
ATOM	1869	ō	LEU		35.232		27.930	1.00	0.00	3A7
ATOM	1870	N	MET	275	35.003		27.521	1.00	0.00	3A7
ATOM	1871	CA	MET	275	35.607		26.211 25.399	1.00	0.00	3A7 3A7
ATOM .	1872 1873	CB CG	MET MET	275 275	35.400 · 33.958 ·		24.962	1.00	0.00	3A7
ATOM	1874	.SD	MET	275	33.857		23.713	1.00	0.00	3A7
ATOM	1875	CE	MET	275	34.315		24.786	1.00	0.00	3A7
ATOM	1876	C	MET	275	37.090 · 37.642 ·		26.286 25.458	1.00	0.00	3A7 3A7
ATOM ATOM	1877 1878	Q N	MET	275 276	37.778		27.305	1.00	0.00	3A7
ATOM	1879	CA	ILE	276	39.215		27.488	1.00	0.00	3A7
MOTA	1880	СВ	ILE	276	39.723		28.575	1.00	0.00	3A7
ATOM	1881		ILE	276	41.140 · 39.717 ·		29.105 28.081	1.00	0.00	3A7 3A7
ATOM ATOM	1882 1883	CD	ILE	276 276	40.767		27.011	1.00	0.00	3A7
ATOM	1884	c	ILE	276	39.615		27.833	1.00	0.00	3A7
MOTA	1885	0	ILE	276	40.701		27.476	1.00	0.00	3A7
ATOM	1886	N CA	ASP ASP	277 277	38.749 39.133		28.548 29.016	1.00	0.00	3A7 3A7
ATOM ATOM	1887 1888	CB	ASP	277	38.914		30.516	1.00	0.00	3A7
ATOM	1889	CG	ASP	277	39.827	-39.210	31.302	1.00	0.00	3A7
ATOM	1890		ASP	277	40.999		30.882	1.00	0.00	3A7 3A7
ATOM ATOM	1891 1892	OD2 C	ASP ASP	277 277	39.351 38.346		32.329 28.476	1.00	0.00	3A7
ATOM	1893	0	ASP	277	38.933		28.164	1.00	0.00	3A7
ATOM	1894	N	SER	278	36.987	-41.031	28.602	1.00	0.00	3A7
ATOM	1895	CA	SER	278	36.186		29.071	1.00	0.00	3A7 3A7
ATOM ATOM	1896 1897	CB OG	SER	278 278	34.677 34.091		29.196 27.961	1.00	0.00	3A7
ATOM	1898	C	SER	278	36.329		28.318	1.00	0.00	3A7
MOTA	1899	0	SER	278	35.567	-43.792	27.399	1.00	0.00	3A7
MOTA	1900	N	GLN	279	37.341	-44.307	28.750	1.00	0.00	3A7

MOTA	1901	CA	GLN	279	37.851	-45.539	28.167	1.00	0.00	3A7
ATOM	1902	СВ	GLN	279	36.793	-46.503	27.561	1.00	0.00	3A7
ATOM	1903	CG	GLN	279	35.768		28.593	1.00	0.00	3A7
ATOM	1904	CD	GLN	279	34.775		27.887	1.00	0.00	3A7
	1905		GLN	279	35.143		27.428	1.00	0.00	3A7
ATOM					33.487		27.805	1.00	0.00	3A7
ATOM	1906		GLN	279			27.116	1.00	0.00	3A7
ATOM	1907	С	GLN	279	38.889					. 3A7
ATOM	1908	0	GLN	279	38.687		25.937	1.00	0.00	
ATOM	1909	N	ASN	280	40.027		27.552		.0.00	. 3A7
ATOM	1910	CA	ASN	280	41.202		26.787	1.00	0.00	3A7
MOTA	1911	CB	ASN	280	42.008		26.209	1.00	0.00	3A7
ATOM	1912	CG	ASN	280	42.430		27.347	1.00	0.00	3A7
MOTA	1913	OD1	ASN	280	41.937	-47.427	27.447	1.00	0.00	3A7
MOTA	1914	ND2	ASN	280	43.366	-45.803	28.213	1.00	0.00	3A7
ATOM	1915	С	ASN	280	40.890	-43.183	25.664	1.00	0.00	3A7
ATOM	1916	0	ASN	280	40.934	-43.532	24.487	1.00	0.00	3A7 ·
ATOM	1917	N	SER	281	40.551	-41.923	26.053	1.00	0.00	3A7
ATOM	1918	CA	SER	281	40.076	-40.803	25.252	1.00	0.00	3A7
ATOM	1919	СВ	SER	281	40.924		23.986	1.00	0.00	3A7
ATOM	1920	OG	SER	281	42.283		24.340	1.00	0.00	3A7
	1921	c	SER	281	38.621		24.837	1.00	0.00	3A7
ATOM					38.131		24.021	1.00	0.00	3A7
ATOM	1922	0	SER	281	37.924		25.342	1.00	0.00	3A7
ATOM	1923	N	LYS	282			24.707	1.00	0.00	3A7
ATOM	1924	CA	LYS	282	36.818					3A7
ATOM	1925	СВ	LYS	282	35.459		24.620	1.00	0.00	
ATOM	1926	CG	LYS	282	34.288		24.294	1.00	0.00	3A7
MOTA	1927	CD		282	32.914		24.590	1.00	0.00	3A7
ATOM	1928	CE	LYS	282	31.744		24.357	1.00	0.00	3A7
ATOM	1929	NZ	LYS	282		-43.746	22.946	1.00	0.00	3A7
ATOM	1930	С	LYS	282	37.194	-43.157	23.334	1.00	0.00	3A7
MOTA	1931	0	LYS	282	37.082		22.364	1.00	0.00	3A7
ATOM	1932	N	ASP	283	37.706	-44.392	23.270	1.00	0.00	3A7
ATOM	1933	CA	ASP	283	38.125	-44.964	22.041	1.00	0.00	3A7
ATOM	1934	СВ	ASP	283	39.663		21.918	1.00	0.00	3A7
ATOM	1935	CG	ASP	283	40.442	-46.002	22.880	1.00	0.00	3A7
ATOM	1936		ASP	283		-46.097	22.672	1.00	0.00	3A7
ATOM	1937		ASP	283	39.853		23.810	1.00	0.00	3A7
ATOM	1938	C	ASP	283	37.352		21.948	1.00	0.00	3A7
ATOM	1939	ŏ	ASP	283		-47.232	22.581	1.00	0.00	3A7
MOTA	1940	N	SER	284	36.258		21.157	1.00	0.00	3A7
		CA	SER	284	35.513		20.782	1.00	0.00	3A7
MOTA	1941				34.115		20.210	1.00	0.00	3A7
MOTA	1942	CB	SER	284		-45.995	19.212	1.00	0.00	3A7
ATOM	1943	OG	SER	284				1.00	0.00	3A7
ATOM	1944	C	SER	284		-48.277	19.834			3A7
MOTA	1945	0	SER	284		-49.180	20.242	1.00	0.00	
MOTA	1946	N	GLU	285		-48.092	18.521	1.00	0.00	3A7
ATOM	1947	CA	GLU	285		-49.081	17.634	1.00	0.00	3A7
ATOM	1948	CB	GLU	285		-49.213	16.369	1.00	0.00	3A7
ATOM	.1949	CG	GLU	285		-47.895	15.591	1.00	0.00	3A7
MOTA	1950	CD	GLU	285		-48.143	14.367	1.00	0.00	3A7
MOTA	1951		GLU	285		-48.527	14.555	1.00	0.00	3A7
ATOM	1952	OE2	GLU	285	35.255	-47.948	13.228	1.00	0.00	3A7
MOTA	1953	С	GLU	285	38.083	-48.834	17.309	1.00	0.00	3A7
MOTA	1954	0	GLU	285	38.621	-49.477	16.447	1.00	0.00	3A7
ATOM	1955	N	THR	286	38.744	-47.901	18.009	1.00	0.00	3A7
ATOM	1956	CA	THR	286	40.099	-47.398	17.894	1.00	0.00	3A7
ATOM	1957	СВ	THR	286	41.251	-48.366	17.728	1.00	0.00	3A7
ATOM	1958		THR	286		-49.460	18.620	1.00	0.00	3A7
ATOM	1959		THR	286		-47.726	18.038	1.00	0.00	3A7
ATOM	1960	C	THR	286		-46.319	16.868	1.00	0.00	3A7
		0	THR	286		-45.529	16.847	1.00	0.00	3A7
ATOM	1961					-46.294	15.904	1.00	0.00	3A7
ATOM	1962	N	HIS	287				1.00	0.00	3A7
ATOM	1963	CA	HIS	287		-45.529	14.676		0.00	3A7
MOTA	1964		HIS	287		-44.452	11.739	1.00		3A7
MOTA	1965	CG	HIS	287		-45.495	12.192	1.00	0.00	
ATOM	1966	СВ	HIS	287		-46.152	13.541	1.00	0.00	3A7
MOTA	1967		HIS	287		-44.903	10.120	1.00	0.00	3A7
MOTA	1968		HIS	287		-45.756	11.189	1.00	0.00	3A7
MOTA	1969	CEl	HIS	287		-44.140	10.497	1.00	0.00	3A7
ATOM	1970	С	HIS	287		-44.107	14.911	1.00	0.00	3A7
ATOM	1971	0	HIS	287	37.679	-43.797	14.904	1.00	0.00	3A7
ATOM	1972	N	LYS	288	39.880	-43.225	15.122	1.00	0.00	3A7

ATOM	1973	CA	LYS	288		39.776	-41.800	15.358	1.00	0.00	3A7
ATOM	1974	CB	LYS	288			-41.036	14.340	1.00	0.00	3A7
ATOM	1975	CG	LYS	288			-41.157	12:.901	1.00	0.00	3A7
ATOM	1976	CD	LYS	288			-40.437	11.877	1.00	0.00 0.00	3A7 3A7
ATOM	1977	CE	LYS	288 · 288			-40.557 -39.909	10.434 10.282	1.00	0.00	3A7 3A7
ATOM ATOM	1978 1979	NZ C	LYS LYS	288			-41.522	16.767	1.00	0.00	3A7
ATOM	1979	ō	LYS	288			-41.380	17.030	1.00	0.00	3A7
MOTA	1981	N	ALA	289			-41.406	17.701	1.00	0.00	3A7
MOTA	1982	CA	ALA	289			-40.977	19.070	1.00	0.00	3A7
ATOM	1983	СВ	ALA	289			-41.545	20.027	1.00	0.00	3A?
ATOM	1984	С	ALA	289			-39.473	19.078	1.00	0.00	3A7
MOTA	1985	0	ALA	289			-38.875	18.128	1.00	0.00	3A7
MOTA	1986	N	LEU	290			-38.812	20.137	1.00	0.00	3A7
MOTA	1987	CA	LEU	290			-37.401	20.081	1.00	0.00	3A7
ATOM	1988	CB	LEU	290			-37.004	21.014	1.00 1.00	0.00	3A7 3A7
MOTA	1989	CG	LEU	290 290			-37.703 -37.512	20.701 21.861	1.00	0.00	3A7
MOTA MOTA	1990 1991		LEU LEU	290			-37.221	19.355	1.00	0.00	3A7
ATOM	1992	C	LEU	290			-36.573	20.350	1.00	0.00	3A7
ATOM	1993	ŏ	LEU	290			-36.642	21.390	1.00	0.00	3A7
ATOM	1994	N	SER	291			-35.731	19.352	1.00	0.00	3A7
ATOM	1995	CA	SER	291		41.954	-34.822	19.363	1.00	0.00	3A7
MOTA	1996	СВ	SER	291			-34.592	17.928	1.00	0.00	3A7
MOTA	1997	OG	SER	291			-34.204	17.030	1.00	0.00	3A7
MOTA	1998	С	SER	291			-33.540	19.957	1.00	0.00	3A7
ATOM	1999	0	SER	291			-33.273	19.991	1.00	0.00	3A7 3A7
MOTA	2000	N	ASP	292			-32.681	20.410 21.064	1.00	0.00	3A7 .
ATOM	2001 2002	CA CB	ASP ASP	292 292			-31.438 -30.745	21.556	1.00	0.00	3A7
ATOM ATOM	2002	CG	ASP	292			-31.647	22.570	1.00	0.00	3A7
ATOM	2003		ASP	292			-31.941	23.629	1.00	0.00	3A7
ATOM	2005		ASP	292			-32.050	22.298	1.00	0.00	3A7
ATOM	2006	С	ASP	292		41.334	-30.471	20.170	1.00	0.00	3A7
ATOM	2007	0	ASP	292			-29.641	20.643	1.00	0.00	3A7
MOTA	2008	N	FEA	293			-30.616	18.834	1.00	0.00	3A7
MOTA	2009	CA	LEU	293			-29.795	17.858	1.00	0.00	3A7 3A7
MOTA	2010	CB		- 293			-29.876	16.490 16.506	1.00	0.00	3A7
ATOM	2011 2012	CG	LEU	293 293			-29.436 -29.663	15.129	1.00	0.00	3A7
ATOM ATOM	2012		LEU	293			-27.976	16.965	1.00	0.00	3A7
ATOM	2014	c	LEU	293			-30.187	17.711	1.00	0.00	, 3A7
ATOM	2015	ŏ	LEU	293			-29.340	17.738	1.00	0.00	3A7
ATOM	2016	N	GLU	294			-31.502	17.619	1.00	0.00	3A7
MOTA	2017	CA	GLU	294		37.722	-31.998	17.504	1.00	0.00	3A7
MOTA	2018	CB	GLU	294			-33.523	17.310	1.00	0.00	3A7
MOTA	2019	CG	GLU	294			-33.957	15.942	1.00	0.00	3A7 3A7
ATOM	2020	CD	GLU	294	•		-35.480	15.850	1.00	0.00	3A7
. ATOM	2021		GLU GLU	294 294	•		-36.040 -36.104	15.905 15.722	1.00	0.00	3A7
ATOM ATOM	2022 2023	C	GLU	294			-31.676	18.723	1.00	0.00	3A7
ATOM	2024	ŏ	GLU	294			-31.192	18.632	1.00	0.00	3A7
ATOM	2025	N	LEU	295			-31.876	19.909	1.00	0.00	3A7
ATOM	2026	CA	LEU	295			-31.573	21.190	1.00	0.00	3A7
MOTA	2027	CB	LEU	295			-31.878	22.313	1.00	0.00	3A7
ATOM	2028	CG	LEU	295			-33.358	22.435	1.00	0.00	3A7 3A7
ATOM	2029		LEU	295			-33.555	23.470 22.783	1.00	0.00	3A7
MOTA	2030		LEU	295 295			-34.206 -30.119	21.312	1.00	0.00	3A7
ATOM ATOM	2031 2032	С 0	LEU	295			-29.765	21.643	1.00	0.00	3A7
ATOM	2032	N	MET	296			-29.212	21.017	1.00	0.00	3A7
ATOM	2034	CA	MET	296			-27.783	21.050	1.00	0.00	3A7
ATOM	2035	СВ	MET	296			-27.070	20.647	1.00	0.00	3A7
ATOM	2036	CG	MET	296			-25.578	20.350	1.00	0.00	3A7
MOTA	2037	SD	MET	296			-24.717	20.404	1.00	0.00	3A7
ATOM	2038	CE	MET	296			-25.540	18.974	1.00	0.00	3A7 3A7
ATOM	2039	C	MET	296			-27.341	20.113	1.00	0.00	3A7 3A7
ATOM	2040	0	MET	296 297			-26.566 -27.882	20.489 18.877	1.00	0.00	3A7
ATOM ATOM	2041 2042	N CA	ALA ALA	297 297			-27.555	17.895	1.00	0.00	3A7
ATOM	2042	CB	ALA	297			-28.182	16.525	1.00	0.00	3A7
ATOM	2044	C	ALA	297			-27.978	18.300	1.00	0.00	3A7
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MOTA	2045	0	ALA	297	32.817	-27.301	17.986	1.00	0.00	3A7
ATOM	2046	N	GLN	298	33.648	-29.071	19.085	1.00	0.00	3A7
MOTA	2047	CA	GLN	298		-29.501	19.640	1.00	0.00	3A7
MOTA	2048	CB	GLN	298		-30.905	20.248	1.00	0.00	3A7
ATOM	2049	CG	GLN	298		-32.025	19.207	1.00	0.00	3A7
MOTA	2050	CD	GLN	298		-33.345	19.922	1.00	0.00	3A7
MOTA	2051		GLN	298		-33.554	20.400	1.00	0.00	3A7
ATOM	2052	NE2	GLN	298		-34.253	19.977	1.00	0.00	3A7 3A7
ATOM	2053	C	GLN	298 298		-28.563 -28.142	20.719 20.728	1.00	0.00	3A7
MOTA MOTA	2054 2055	O N	GLN SER	299		-28.160	21.630	1.00	0.00	3A7
ATOM	2056	CA	SER	299		-27.222	22.690	1.00	0.00	3A7
ATOM	2057	СВ	SER	299		-27.023	23.597	1.00	0.00	3A7
ATOM	2058	OG	SER	299		-28.269	24.141	1.00	0.00	3A7
MOTA	2059	C	SER	299		-25.874	22.158	1.00	0.00	3A7
ATOM	2060	0	SER	299		-25.252	22.698		0.00	3A7
MOTA	2061	N	ILE	300		-25.399	21.047	1.00	0.00.	3A7
ATOM	2062	CA	ILE	300		-24.170	20.361	1.00	0.00	3A7
ATOM	2063	CB	ILE	300		-23.832	19.229	1.00	0.00	3A7 3A7
ATOM	2064		ILE	300		-22.603 -23.560	18.412 19.774	1.00	0.00	3A7
ATOM ATOM	2065 2066	CG1	ILE	300 300		-23.539	18.691	1.00	0.00	3A7
ATOM	2067	C	ILE	300		-24.293	19.764	1.00	0.00	3A7
ATOM	2068	ŏ	ILE	300		-23.398	19.914	1.00	0.00	3A7
ATOM	2069	N	ILE	301		-25.431	19.092	1.00	0.00	3A7
MOTA	2070	CA	ILE	301		-25.676	18.455	1.00	0.00	3A7
MOTA	2071	CB	ILE	301	29.475	-26.900	17.553	1.00	0.00	3A7
MOTA	2072	CG2	ILE	301		-27.772	17.525	1.00	0.00	3A7
ATOM	2073	CG1	ILE	301		-26.460	16.091	1.00	0.00	3A7
ATOM	2074	CD	ILE	301		-25.647	15.869	1.00	0.00	3A7
ATOM	2075	C	ILE	301 301		-25.792 -25.379	19.465 19.205	1.00	0.00	3A7 3A7
ATOM ATOM	2076 2077	O N	ILE Phe	302		-26.318	20.673	1.00	0.00	3A7
ATOM	2078	CA	PHE	302		-26.507	21.709	1.00	0.00	3A7
ATOM	2079	СВ	PHE	302		-27.306	22.878	1.00	0.00	3A7
MOTA	2080	CG	PHE	302	28.239	-28.790	22.660	1.00	0.00	3A7
MOTA	2081	CD1	PHE	302 ·	28.348	-29.335	21.379	1.00	0.00	3A7
ATOM	2082	CD2	PHE	302		-29.577	23.757	1.00	0.00	3A7
MOTA	2083		PHE	302		-30.584	21.188	1.00	0.00	3A7
MOTA	2084		PHE	302		-30.829	23.567	1.00	0.00	3A7
ATOM	2085	CZ	PHE	302		-31.311 -25.150	22.282 22.252	1.00	0.00	3A7 3A7
ATOM ATOM	2086 2087	С О	PHE	302 302		-24.892	22.478	1.00	0.00	3A7
ATOM	2088	N	ILE	303		-24.221	22.452	1.00	0.00	3A7
ATOM	2089	CA	ILE	303		-22.889	22.966	1.00	0.00	3A7
ATOM	2090	СВ	ILE	303		-22.188	23.539	1.00	0.00	3A7
ATOM	2091	CG2	ILE	303	28.716	-20.768	24.038	1.00	0.00	3A7
MOTA	2092	CG1	ILE	303		-23.043	24.700	1.00	0.00	3A7
MOTA	2093	CD	ILE .	303		-22.513	25.280	1.00	0.00	3A7
MOTA	2094	C	ILE	303		-22.030	21.914	1.00	0.00	3A7
MOTA	2095	0	ILE PHE	303 304		-21.376 -22.042	22.173 20.671	1.00	0.00	3A7 3A7
ATOM ATOM	2096 2097	N CA	PHE	304		-21.301	19.548	1.00	0.00	3A7
ATOM	2098	СВ	PHE	304		-21.579	18.314		0.00	3A7
ATOM	2099	CG	PHE	304		-20.996	16.996	1.00	0.00	3A7
MOTA	2100		PHE	304		-19.644	16.704	1.00	0.00	3A7
MOTA	2101		PHÉ	304	27.091	-21.829	16.036	1.00	0.00	3A7
ATOM	2102		PHE	304		-19.134	15.472	1.00	0.00	3A7
MOTA	2103		PHE	304		-21.320	14.811	1.00	0.00	3A7
ATOM	2104	CZ	PHE	304		-19.970	14.526	1.00	0.00	3A7
ATOM	2105	C	PHE	304 304		-21.649 -20.780	19.207 19.129	1.00	0.00	3A7 3A7
MOTA MOTA	2106 2107	о И	PHE	304 305		-22.954	19.129	1.00	0.00	3A7
ATOM	2108	CA	ALA	305		-23.428	18.672	1.00	0.00	3A7
ATOM	2109	СВ	ALA	305		-24.883	18.216	1.00	0.00	3A7
ATOM	2110	C	ALA	305		-23.354	19.820	1.00	0.00	3A7
ATOM	2111	0	ALA	305		-23.132	19.620	1.00	0.00	3A7
ATOM	2112	N	GLY	306		-23.533	21.051	1.00	0.00	3A7
ATOM	2113	CA	GLY	306		-23.642	22.219	1.00	0.00	3A7
ATOM	2114	Ç	GLY .	306		-22.346	22.888	1.00	0.00	3A7
MOTA	2115	Й	GLY	306 307		-22.258 -21.285	23.561 22.742	1.00	0.00	3A7 3A7
MOTA	2116	4.4	TYR	,	20.000	Z Z. U.J	~~	4.00		JA!

ATOM	2117	CA	TYR	307	23.134 -20	.054	23.474	1.00	0.00	3A7
ATOM	2118	СВ	TYR	307	24.473 -19		23.690	1.00	0.00	3A7
ATOM	2119	CG	TYR	307	24.492 -17	.764	23.545	1.00	0.00	3A7
MOTA	2120	CD1	TYR	307	23.675 -16		24.308	1.00	0.00	3A7
MOTA	2121		TYR	307	25.364 -17		22.621	1.00	0.00	3A7
ATOM	2122		TYR	307	23.720 -15		24.144	1.00	0.00	3A7
MOTA	2123		TYR	307	25.420 -15		22.460	1.00	0.00	3A7 3A7
MOTA	2124	cz	TYR	307	24.595 -14 24.653 -13		23.222 23.066	1.00	0.00 0.00	3A7
ATOM	2125	OH	TYR TYR	307 307	22.056 -19		22.841	1.00	0.00	3A7
MOTA MOTA	2126 2127	С 0	TYR	307	21.092 -18		23.498	1.00	0.00	3A7
ATOM	2128	N	GLU	308	22.222 -18		21.552	1.00	0.00	3A7
ATOM	2129	CA	GLU	308	21.442 -17		20.875	1.00	0.00	3A7
ATOM	2130	СВ	GLU	308	22.048 -17	. 593	19.488	1.00	0.00	3A7
ATOM	2131	CG	GLU	308	22.280 -18	.862	18.631	1.00	0.00	3A7
ATOM	2132	CD	GLU	308	23.057 -18		17.347	1.00	0.00	3A7
ATOM	2133		GLU	308	23.277 -17		17.030	1.00	0.00	3A7
ATOM	2134		GLU	308	23.430 -19		16.657	1.00	0.00	3A7
MOTA	2135	С	GLU	308	20.007 -18		20.661	1.00	0.00	3A7 3A7
ATOM	2136	0	GLU	308	19.119 -17		20.814	1.00	0.00	3A7 3A7
ATOM	2137	N	THR	309 309	19.741 -19 18.413 -20		20.080	1.00	0.00	3A7
ATOM ATOM	2138 2139	CA CB	THR	309	18.504 -21		19.437	1.00	0.00	3A7
ATOM	2140		THR	309	17.244 -21		18.974	1.00	0.00	3A7
ATOM	2141		THR	309	19.256 -22		20.330	1.00	0.00	3A7
ATOM	2142	C	THR	309	17.592 -20		21.350	1.00	0.00	3A7
ATOM	2143	0	THR	309	16.436 -19		21.350	1.00	0.00	3A7
ATOM	2144	N	THR	310	18.187 -20		22.480	1.00	0.00	3A7
ATOM	2145	CA	THR	310	17.519 -20		23.760	1.00	0.00	3A7
MOTA	2146	CB	THR	310	18.271 -21		24.744	1.00	0.00	3A7
ATOM	2147		THR	310	18.739 -22		24.101	1.00	0.00	3A7 3A7
ATOM	2148 2149		THR	310 310	17.383 -21 17.233 -19		25.943 24.344	1.00	0.00	3A7
ATOM ATOM	2149	C O	THR	310	16.168 -18		24.914	1.00	0.00	3A7
ATOM	2151	N	SER	311	18.147 -18		24.167	1.00	0.00	3A7
ATOM	2152	·CA	SER	311	17.925 -16		24.659	1.00	0.00	3A7
ATOM	2153	СВ	SER	311	19.171 -15	.993	24.620	1.00	0.00	3A7
ATOM	2154	OG	SER	311	20.346 -16	.710	24.906	1.00	0.00	3A7
ATOM	2155	С	SER	311	16.857 -16		23.854	1.00	0.00	3A7
ATOM	2156	0	SER	311	15.998 -15		24.407	1.00	0.00	3A7
ATOM	2157	N	SER	312	16.848 -16		22.505	1.00	0.00	3A7 3A7
ATOM	2158	CA	SER	312	15.858 -15 16.203 -15		21.625	1.00	0.00	3A7
ATOM ATOM	2159 2160	CB OG	SER SER	312 312	16.398 -17		19.751	1.00	0.00	3A7
ATOM	2161	c	SER	312	14.473 -16		21.903	1.00		3A7
ATOM	2162	ō	SER	312	13.477 -15		21.718	1.00	0.00	3A7
ATOM	2163	N	VAL	313	14.376 -17		22.376	1.00	0.00	3A7
ATOM	2164	CA	VAL	313	. 13.115 -18	.232	22.678	1.00	0.00	3A7
MOTA	2165	ĊВ	VAL	313	13.262 -19		22.736	1.00	0.00	3A7
MOTA	2166		VAL	313	12.003 -20		23.260	1.00	0.00	3A7
ATOM	2167		VAL	313	13.426 -20		21.263	1.00	0.00	3A7
ATOM	2168	C	VAL	313	12.555 -17		23.971	1.00	0.00	3A7 · 3A7
ATOM ATOM	2169 2170	O N	VAL	313 314	11.368 -17 13.406 -17		24.059	1.00	0.00	3A7
ATOM	2171	CA	LEU	314	13.003 -16		26.283	1.00	0.00	3A7
ATOM	2172	CB	LEU	314	14.178 -17		27.279	1.00	0.00	3A7
ATOM	2173	CG	LEU	314	14.712 -18		27.608	1.00	0.00	3A7
ATOM	2174		LEU	314	16.160 -18	.400	28.135	1.00	0.00	3A7
ATOM	2175		LEU	314	13.817 -19	.188	28.604	1.00	0.00	3A7
ATOM	2176	С	LEU	314	12.519 -15		26.181	1.00	0.00	3A7
ATOM	2177	0	LEU	314	11.490 -15		26.736	1.00	0.00	3A7
ATOM	2178	N	SER	315	13.252 -14		25.411	1.00	0.00	3A7
ATOM	2179	CA	SER	315	12.914 -13 14.033 -12		25.165 24.406	1.00	0.00	3A7 3A7
ATOM	2180 2181	CB OG	SER	315 315	15.234 -12		25.166	1.00	0.00	3A7
ATOM ATOM	2181	C	SER SER	315	11.625 -13		24.374	1.00	0.00	3A7
MOTA	2183	ŏ	SER	315	10.814 -12		24.676	1.00	0.00	3A7
ATOM	2184	N	PHE	316	11.391 -14		23.358	1.00	0.00	3A7
ATOM	2185	CA	PHE	316	10.164 -14		22.587	1.00	0.00	3A7
ATOM	2186	СВ	PHE	316	10.264 -14		21.289	1.00	0.00	3A7
ATOM	2187	CG	PHE	316	10.697 -14		20.108	1.00	0.00	3A7
ATOM	2188	CD1	PHE	316	11.810 -14	1.439	19.342	1.00	0.00	3A7

ATOM	2189	CD2	PHE	316	9,933	-12.985	19.709	1.00	0.00	3A7
ATOM	2190	CEI		316		-13.699	18.217	1.00	0.00	3A7
ATOM	2191	CE2		316		-12.246	18.582	1.00	0.00	3A7
ATOM	2192	CZ	PHE	316		-12.600	17.837	1.00	0.00	3A7
MOTA	2193	C	PHE	316		-14.618	23.406	1.00	0.00	3A7
	2194	Ö	PHE	316		-14.133	23.296	1.00	0.00	3A7
MOTA			ILE	317		-15.617	24.306	1.00	0.00	3A7
MOTA	2195	N				-16.171	25.144	1.00	0.00	3A7
ATOM	2196	CA	ILE	317		-17.418	26.022	1.00	0.00	3A7
ATOM	2197	CB	ILE	317		-17.454	27.357	1.00	0.00	3A7
ATOM	2198	CG2		317			25.331	1.00	0.00	3A7
ATOM	2199	CG1		317		-18.749		1.00	0.00	3A7
ATOM	2200	CD	ILE	317		-19.340	24.419		0.00	3A7
MOTA	2201	С	ILE	317		-15.117	26.091	1.00		3A7
ATOM	2202	0	ILE	317		-14.997	26.274	1.00	0.00	3A7
ATOM	2203	N	ILE	318		-14.313	26.715	1.00	0.00	3A7
ATOM	2204	CA	ILE	318		-13.252	27.635	1.00	0.00	
ATOM	2205	CB	ILE	318		-12.624	28.274	1.00	0.00	3A7
MOTA	2206	CG2	ILE	318		-11.357	29.092	1.00	0.00	3A7
MOTA	2207	CG1	ILE	318		-13.689	29.181	1.00	0.00	3A7
ATOM	2208	CD	ILE	318	11.481	-13.295	29.665	1.00	0.00	3A7
ATOM	2209	С	ILE	318	7.339	-12.213	26.942	1.00	0.00	3A7
ATOM	2210	0	ILE	318	6.296	-11.802	27.441	1.00	0.00	3A7
ATOM	2211	N	TYR	319	7.731	-11.823	25.716	1.00	0.00	3A7
ATOM	2212	CA	TYR	319	6.987	-10.893	24.906	1.00	0.00	3A7
ATOM	2213	CB	TYR	319	7.729	-10.658	23.571	1.00	0.00	3A7
ATOM	2214	CG	TYR	319	6.940	-9.879	22.557	1.00	0.00	3A7
ATOM	2215		TYR	319	6.414	-8.628	22.863	1.00	0.00	3A7
ATOM	2216		TYR	319	6.693	-10.438	21.301	1.00	0.00	3A7
ATOM	2217		TYR	319	5.597	-7.976	21.949	1.00	0.00	3A7
ATOM	2218		TYR	319	5.898	-9.773	20.375	1.00	0.00	3A7
ATOM	2219	CZ	TYR	319	5.336	-8.544	20.704	1.00	0.00	3A7
ATOM	2220	OH	TYR	319	4.491	-7.887	19.783	1.00	0.00	3A7
ATOM	2221	c	TYR	319		-11.359	24.631	1.00	0.00	3A7
ATOM	2222	ŏ	TYR	319		-10.588	24.752	1.00	0.00	3A7
ATOM	2223	N	GLU	320		-12.651	24.277	1.00	0.00	3A7
ATOM	2224	CA	GLU	320		-13.205	23.952	1.00	0.00	3A7
ATOM	2225	CB	GLU	320		-14.545	23.220	1.00	0.00	· 3A7
	2226	CG	GLU	320		-14.416	21.829	1.00	0.00	3A7
MOTA MOTA	2227	CD	GLU	320		-13.768	20.915	1.00	0.00	3A7
	2228		GLU	320		-12.634	20.435	1.00	0.00	3A7
ATOM	2229		GLU	320		-14.384	20.681	1.00	0.00	3A7
MOTA	2230		GLU	320		-13.345	25.140	1.00	0.00	3A7
ATOM		C		320		-13.087	25.041	1.00	0.00	3A7
ATOM	2231	0	GLU	321		-13.705	26.321	1.00	0.00	3A7
ATOM	2232	N	LEU			-13.799	27.537	1.00	0.00	3A7
ATOM	2233	CA	LEU	321				1.00	0.00	3A7
ATOM	2234	CB	LEU	321		-14.427 -15.941	28.662 28.472	1.00	0.00	3A7
ATOM	2235	CG	LEU	321				1.00	0.00	3A7
ATOM	2236		LEU	321		-16.456	29.453			3A7
ATOM	,2237		LEU	321		-16.706	28.641	1.00	0.00	3A7
ATOM	2238	C	LEU	321		-12.447	28.007	1.00	0.00	3A7 3A7
ATOM	2239	0	LEU	321		-12.302	28.509	1.00	0.00	3A7
ATOM	2240	N	ALA	322		-11.421	27.837	1.00	0.00	3A7 3A7
ATOM	2241	CA	ALA	322		-10.068	28.220	1.00	0.00	
ATOM	2242	CB	ALA	322		-9.229		1.00		3A7
ATOM	2243	С	ALA	322	2.044	-9.469	27.279	1.00	0.00	3A7
ATOM	2244	0	ALA	322	1.166		27.668	1.00	0.00	3A7
ATOM	2245	N	THR	323	2.110	-9.863	25.996	1.00	0.00	3A7
MOTA	2246	CA	THR	323	1.174	-9.402	25.006	1.00	0.00	3A7
ATOM	2247	CB	THR	323	1.714	-9.509	23.612	1.00	0.00	3A7
ATOM	2248	0G1	THR	323	2.224	-10.786	23.282	1.00	0.00	3A7
ATOM	2249	ÇG2	THR	323	2.782	-8.417	23.418	1.00	0.00	3A7
ATOM	2250	С	THR	323		-10.105	25.063	1.00	0.00	3A7
ATOM	2251	0	THR	323	-1.132		24.486	1.00	0.00	3A7
ATOM	2252	N	HIS	324	-0.258	-11.241	25.774	1.00	0.00	3A7
ATOM	2253	CA	HIS	324	-1.475	-12.018	25.882	1.00	0.00	3A7
ATOM	2254	ND1	HIS	324		-12.554	22.767	1.00	0.00	3A7
MOTA	2255	CG	HIS	324	-1.279	-13.139	23.576	1.00	0.00	3A7
ATOM	2256	СВ	HIS	324	-1.248	-13.311	25.087	1.00	0.00	3A7
ATOM	2257		HIS	324	-0.359	-12.447	21.617	1.00	0.00	3A7
ATOM	2258		HIS	324		-13.016	22.856	1.00	0.00	3A7
MOTA	2259		HIS	324		-12.187	21.610	1.00	0.00	3A7
ATOM	2260	c	HIS	324		-12.327	27.334	1.00	0.00	3A7
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ATOM	2261	0	HIS	324	-1.410	-13.448	27.764	1.00	0.00	3A7
ATOM	2262	N	PRO	325		-11.398	28.139	1.00	0.00	3A7
	2263	CA	PRO	325		-11.530	29.587	1.00	0.00	3A7
ATOM							27.697	1.00	0.00	3A7
ATOM	2264	CD	PRO	325		-10.073			0.00	3A7
MOTA	2265	СВ	PRO	325		-10.217	30.049	1.00		
ATOM	2266	CG	PRO	325	-2.634	-9.212	28.959	1.00	0.00	3A7
ATOM	2267	С	PRO	325	-3.219	-12.703	30.001	1.00	0.00	3A7
ATOM	2268	0	PRO	325	-2.994	-13.255	31.072	1.00	0.00	3A7
ATOM	2269	N	ASP	326		-13.144	29.162	1.00	0.00	3A7
					-5.016		29.448	1.00	0.00	3A7
ATOM	2270	CA	ASP	326			28.372	1.00	0.00	3A7
MOTA	2271	СВ	ASP	326		-14.480				
MOTA	2272	CG	ASP	326		-13.305	28.363	1.00	0.00	3A7
ATOM	2273	OD1	ASP	326	-7.016	-12.435	29.271	1.00	0.00	3A7
ATOM	2274	OD2	ASP	326	-7.946	-13.276	27.437	1.00	0.00	3A7
ATOM	2275	С	ASP	326	-4.191	-15.557	29.518	1.00	0.00	3A7
ATOM	2276	ŏ	ASP	326		-16.408	30.379	1.00	0.00	3A7
				327		-15.680	28.617	1.00	0.00	3A7
ATOM	2277	N	VAL					1.00	0.00	3A7
ATOM	2278	CA	VAL	327		-16.822	28.551			
ATOM	2279	CB	VAL	327		-16.855	27.249	1.00	0.00	3A7
ATOM	2280	CG1	VAL	327	-0.634	-18.114	27.189	1.00	0.00	3A7
ATOM	2281	CG2	VAL	327	-2.526	-16.830	26.078	1.00	0.00	3A7
ATOM	2282	С	VAL	327	-1.357	-16.811	29.718	1.00	0.00	3A7
ATOM	2283	ŏ	VAL	327		-17.833	30.353	1.00	0.00	3A7
						-15.622	30.057	1.00	0.00	3A7
MOTA	2284	N	GLN	328					0.00	3A7
MOTA	2285	CA	GLN	328		-15.440	31.190	1.00		
ATOM	2286	СB	GLN	328		-13.994	31.280	1.00	0.00	3A7
ATOM	2287	CG	GLN	328	1.927	-13.874	31.956	1.00	0.00	3A 7
MOTA	2288	CD	GLN	328	2.430	-12.432	31.850	1.00	0.00	3A7
ATOM	2289	OE1	GLN	328	1.677	-11.512	31.507	1.00	0.00	3A7
ATOM	2290		GLN	328		-12.247	32.162	1.00	0.00	3A7
				328	_	-15.809	32.500	1.00	0.00	3A7
ATOM	2291	C	GLN						0.00	3A7
ATOM	2292	0	GLN	328		-16.448	33.339	1.00		
MOTA	2293	N	GLN	329		-15.438	32.692	1.00	0.00	3A7
MOTA	2294	CA	GLN	329	-2.599	-15.749	33.879	1.00	0.00	3A7
ATOM	2295	CB	GLN	329	-3.961	-15.032	33.870	1.00	0.00	3A7
ATOM	2296	CG	GLN	329	3.832	-13.525	34.148	1.00	0.00	3A7
ATOM	2297	CD	GLN	329		-12.882	34.023	1.00	0.00	3A7 -
	2298		GLN	329		-13.175	34.813	1.00	0.00	3A7
ATOM						-11.987	33.000	1.00	0.00	3A7
ATOM	2299		GLN	329						3A7
ATOM	2300	С	GLN	329		-17.226	34.022	1.00	0.00	
MOTA	2301	0	GLN	329		-17.780	35.102	1.00	0.00	3A7
MOTA	2302	N	LYS	330	-3.153	-17.913	32.907	1.00	0.00	3A7
ATOM	2303	CA	LYS	330	-3.370	-19.343	32.883	1.00	0.00	3A7
ATOM	2304	СВ	LYS	330	-3.917	-19.754	31.503	1.00	0.00	3A7
ATOM	2305	CG	LYS	330		-21.169	31.446	1.00	0.00	3A7
	2306	CD	LYS	330		-21.428	30.124	1.00	0.00	3A7
ATOM								1.00	0.00	3A7
MOTA	2307	CE	LYS	330		-22.799	30.054			
MOTA	2308	NZ	LYS	330		-22.943	31.113	1.00	0.00	3A7
. ATOM	2309	С	LYS	330	2.097	-20.090	33.241	1.00	0.00	3A7
ATOM	2310	0	LYS	330	-2.090	-21.027	34.040	1.00	0.00	3A7
ATOM	2311	N	VAL	331	-0.946	-19.618	32.704	1.00	0.00	3A7
ATOM	2312	CA	VAL	331	0.363	-20.189	32.957	1.00	0.00	3A7
ATOM	2313	СВ	VAL	331		-19.605	32.030	1.00	0.00	3A7
			VAL	331		-20.076	32.382	1.00	0.00	3A7
ATOM	2314								0.00	3A7
MOTA	2315		VAL	331		-20.072	30.601	1.00		
ATOM	2316	C	VAL	331		-19.992	34.390	1.00	0.00	3A7
ATOM	2317	0	VAL	331		-20.919	35.023	1.00	0.00	3A7
ATOM	2318	N	GLN	332	0.561	-18.783	34.951	1.00	0.00	3A 7
ATOM	2319	CA	GLN	332	0.896	-18.455	36.319	1.00	0.00	3A7
ATOM	2320	CB	GLN	332		-16.968	36.628	1.00	0.00	3A7
ATOM	2321	CG	GLN	332		-16.072	36.011	1.00	0.00	3A7
							36.311	1.00	0.00	3A7
ATOM	2322	CD	GLN	332		-14.601				
ATOM	2323		GLN	332		-13.947	37.057	1.00	0.00	3A7
ATOM	2324	NE2	GLN	332		-14.079	35.701	1.00	0.00	3A7
ATOM	2325	С	GLN	332	0.082	-19.234	37.311	1.00	0.00	3A7
ATOM	2326	0	GLN	332	0.592	-19.634	38.351	1.00	0.00	3A7
ATOM	2327	N	LYS	333		-19.512	36.991	1.00	0.00	3A7
ATOM	232B	CA	LYS	333		-20.320	37.797	1.00	0.00	3A7
							37.204	1.00	0.00	3A7
ATOM	2329	CB	LYS	333		-20.312				3A7
ATOM	2330	CG	LYS	333		-21.052	38.035	1.00	0.00	
MOTA	2331	CD	LYS	333		-20.945	37.441	1.00	0.00	3A7
MOTA	2332	CE	LYS	333	-6.125	-21.617	36.068	1.00	0.00	3A7

ATOM	2333	NZ	LYS	333	-7.518	-21.516	35.576	1.00	0.00	3A7
ATOM	2334	С	LYS	333	-1.600	-21.746	37.882	1.00	0.00	3A7
ATOM	2335	ō	LYS	333		-22.344	38.954	1.00	0.00	3A7
				334		-22.295	36.728	1.00	0.00	3A7
ATOM	2336	N	GLU						0.00	3A7
ATOM	2337	CA	GLU	334		-23.579	36.649	1.00		
ATOM	2338	СВ	GLU	334		-23.952	35.224	1.00	0.00	3A7
MOTA	2339	CG	GLU	334	-0.038	-25.481	35.122	1.00	0.00	3A7
ATOM	2340	CD	GLU	334	0.087	-25.922	33.672	1.00	0.00	3A7
ATOM	2341	OE1	GLU	334		-26.779	33.251	1.00	0.00	3A7
ATOM	2342		GLU	334		-25.424	32.971	1.00	0.00	3A7
		C	GLU	334		-23.722	37.472	1.00	0.00	3A7
MOTA	2343							1.00	0.00	3A7
ATOM	2344	0	GLU	334		-24.667	38.236			
MOTA	2345	N	ILE	335		-22.744	37.370	1.00	0.00	3A7
ATOM	2346	CA	ILE	335		-22.692	38.098	1.00	0.00	3A7
MOTA	2347	CB	ILE	335	3.672	-21.474	37.679	1.00	0.00	3A7
ATOM	2348	CG2	ILE	335	4.884	-21.230	38.599	1.00	0.00	3A7
ATOM	2349		ILE	335		-21.660	36.215	1.00	0.00	3A7
ATOM	2350	CD	ILE	335		-20.360	35.597	1.00	0.00	3A7
						-22.684	39.587	1.00	0.00	3A7
MOTA	2351	C	ILE	335						3A7
MOTA	2352	0	ILE	335		-23.480	40.320	1.00	0.00	
ATOM	2353	N	ASP	336		-21.822	40.071	1.00	0.00	3A7
MOTA	2354	CA	ASP	336	1.416	-21.706	41.476	1.00	0.00	3A7
MOTA	2355	CB	ASP	336	0.411	-20.565	41.750	1.00	0.00	3A7
ATOM	2356	CG	ASP	336	1.021	-19.199	41.420	1.00	0.00	3A7
ATOM	2357		ASP	336		-19.127	41.123	1.00	0.00	3A7
			ASP			-18.199	41.470	1.00	0.00	3A7
MOTA	2358			336				1.00	0.00	3A7
MOTA	2359	С	ASP	336		-22.996	42.010			3A7
ATOM	2360	0	ASP	336		-23.420	43.106	1.00	0.00	
ATOM	2361	N	THR	337		-23.674	41.213	1.00	0.00	3A7
MOTA	2362	CA	THR	337	-0.701	-24.903	41.571	1.00	0.00	3A7
ATOM	2363	СВ	THR	337	-1.854	-25.156	40.609	1.00	0.00	3A7
ATOM	2364		THR	337	-2.791	-24.092	40.721	1.00	0.00	3A7
ATOM	2365		THR	337		-26.473	40.896	1.00	0.00	3A7
ATOM	2366	C	THR	337		-26.114	41.595	1.00	0.00	3A7
						-27.000	42.433	1.00	0.00	3A7
ATOM	2367	0	THR	337						3A7
MOTA	2368	N	VAL	338		-26.189	40.667	1.00	0.00	
MOTA	2369	CA	VAL	338		-27.349	40.503	1.00	0.00	3A7
MOTA	2370	CB	VAL	338	2.466	-27.564	39.051	1.00	0.00	7א3
MOTA	2371	CG1	VAL	338	3.403	-28.783	38.900	1.00	0.00	3A7
ATOM	2372	CG2	VAL	338	1.182	-27.789	38.226	1.00	0.00	3A7
ATOM	2373	С	VAL	338		-27.232	41.404	1.00	0.00	3A7
ATOM	2374	ō	VAL	338		-28.178	42.113	1.00	0.00	3A7
			LEU	339		-26.065	41.421	1.00	0.00	3A7
ATOM	2375	N				-25.835		1.00	0.00	3A7
MOTA	2376	CA	LEU	339			42.331			
MOTA	2377	CB	LEU	339		-25.014	41.736	1.00	0.00	3A7
ATOM	2378	CG	LEU	339		-25.819	40.766	1.00	0.00	. 3A7
MOTA	2379	CD1	LEU	339	8.159	-24.904	40.176	1.00	0.00	3A7
ATOM	2380	CD2	LEU	339	7.715	-27.051	41.439	1.00	0.00	3A7
ATOM	2381	С	LEU	339	4.552	-25.038	43.521	1.00	0.00	3A7
ATOM	2382	Ō	LEU	339	4.197	-23.878	43.325	1.00	0.00	3A7
ATOM	2383	N	PRO	340		-25.565	44.752	1.00	0.00	3A7
				340		-24.851	45.907	1.00	0.00	3A7
MOTA	2384	CA	PRO				45.025	1.00	0.00	3A7
ATOM	2385	CD	PRO	340		-26.986				
ATOM	2386	CB	PRO	340		-25.968	46.840	1.00	0.00	3A7
MOTA	2387	CG	PRO	340		-27.154	46.523	1.00	0.00	3A7
ATOM	2388	С	PRO	340		-24.042	46.550	1.00	0.00	3A7
ATOM	2389	0	PRO	340	6.241	-24.463	46.512	1.00	0.00	3A7
ATOM	2390	N	ASN	341	4.716	-22.893	47.182	1.00	0.00	3a7
ATOM	2391	CA	ASN	341		-22.073	48.065	1.00	0.00	3A7
						-22.872	49.244	1.00	0.00	3A7
ATOM	2392	CB	ASN	341			50.023	1.00	0.00	3A7
ATOM	2393	CG	ASN	341		-23.614				3A7
MOTA	2394		ASN	341		-24.850	50.059	1.00	0.00	
ATOM	2395	ND2	ASN	341		-22.826	50.663	1.00	0.00	3A7
ATOM	2396	С	ASN	341		-21.330	47.312	1.00	0.00	3A7
ATOM	2397	o	ASN	3.41	6.423	-20.897	.46.178	1.00	0.00	3A7
ATOM	2398	N	LYS	342		-21.175	47.953	1.00	0.00	3A7
ATOM	2399	CA	LYS	342		-20.529	47.396	1.00	0.00	3A7
	2400		LYS	342		-19.456	48.339	1.00	0.00	
ATOM		CB					48.647	1.00	0.00	3A7
MOTA	2401	CG	LYS	342		-18.309				3A7
MOTA	2402	CD	LYS	342		-17.205	49.527	1.00	0.00	
MOTA	2403	CE	LYS	342		-17.674	50.944	1.00	0.00	3A7
MOTA	2404	NZ	LYS	342	10.133	-16.560	51.741	1.00	0.00	3A7

ATOM	2405	С	LYS	342	10.016	-21.594	47.146	1.00	0.00	3A7
ATOM	2406	0	LYS	342		-21.442	47.515	1.00	0.00	3A7
ATOM	2407	.N	ALA	343		-22.711	46.501	1.00	0.00	3A7
ATOM	2408	CA	ALA	343		-23.839	46.171	1.00	0.00	3A7
ATOM	2409	CB	ALA	343	9.750		46.468	1.00	0.00	3A7 3A7
ATOM	2410	C	ALA	343 343		-23.763 -23.520	44.700 43.911	1.00	0.00	3A7
MOTA MOTA	2411 2412	N N	ALA PRO	344		-24.000	44.274	1.00	0.00	3A7
ATOM	2413	CA	PRO	344		-24.110	42.875	1.00	0.00	3A7
ATOM	2414	CD	PRO	344		-23.771	45.118	1.00	0.00	3A7
ATOM	2415	CB	PRO	344	13.894	-24.072	42.880	1.00	0.00	3A7
MOTA	2416	CG	PRO	344		-23.318	44.160	1.00	0.00	3A7
ATOM	2417	C	PRO	344		-25.414	42.274	1.00	0.00	3A7 3A7
ATOM	2418	0	PRO	344		-26.289 -25.589	43.033 40.953	1.00	0.00	3A7
ATOM ATOM	2419 2420	N CA	PRO	345 345		-26.737	40.270	1.00	0.00	3A7
ATOM	2421	CD	PRO	345		-24.479	40.043	1.00	0.00	3A7
ATOM	2422	СВ	PRO	345		-26.382	38.778	1.00	0.00	3A7
ATOM	2423	CG	PRO	345		-24.857	38.731	1.00	0.00	3A7
MOTA	2424	С	PRO	345		-27.996	40.521	1.00	0.00	3A7
MOTA	2425	0	PRO	345		-27.934	40.723	1.00	0.00	3A7 3A7
ATOM	2426 2427	N CA	THR	346 346		-29.156 -30.434	40.428 40.286	1.00	0.00	3A7
MOTA MOTA	2428	CB	THR	346		-31.522	41.180	1.00	0.00	3A7
ATOM	2429		THR	346		-31.633	41.047	1.00	0.00	3A7
ATOM	2430		THR	346		-31.183	42.644	1.00	0.00	3A7
ATOM	2431	С	THR	346		-30.751	38.827	1.00	0.00	3A7
MOTA	2432	0	THR	346		-29.983	38.054	1.00	0.00	3A7
ATOM	2433	N	TYR	347		-31.922	38.405 37.022	1.00	0.00	3A7 3A7
ATOM ATOM	2434 2435	CA CB	TYR TYR	347 347		-32.298 -33.383	36.599	1.00	0.00	3A7
MOTA	2436	CG	TYR	347		-34.221	37.758	1.00	0.00	3A7
ATOM	2437		TYR	347		-35.455	38.007	1.00	0.00	3A7
MOTA	2438	CD2	TYR	347		-33.809	38.584	1.00	0.00	3A7
MOTA	2439		TYR	347		-36.258	39.060	1.00	0.00	3A7
ATOM	2440		TYR	347		-34.609	39.638 39.877	1.00	0.00	3A7 3A7
ATOM ATOM	2441 2442	CZ OH	TYR TYR	347 347		-35.835 -36.649	40.945	1.00	0.00	3A7
ATOM	2443	C	TYR	347		-32.842	36.741	1.00	0.00	3A7
MOTA	2444	Ō	TYR	347		-32.653	35.655	1.00	0.00	3A7
ATOM	2445	N	ASP	348	10.354	-33.487	37.746	1.00	0.00	3A7
MOTA	2446	CA	ASP	348		-34.072	37.677	1.00	0.00	3A7
ATOM	2447	CB	ASP			-34.785 -35.950	38.996 39.163	1.00	0.00	3A7 3A7
ATOM ATOM	2448 2449	CG	ASP ASP	348 348		-36.846	38.277	1.00	0.00	3A7
ATOM	2450		ASP	348		-35.959	40.167	1.00	0.00	3A7
ATOM	2451	С	ASP	348		-33.064	37.424	1.00	0.00	3A7
ATOM	2452	0	ASP	348		-33.393	36.890	1.00	0.00	3A7
MOTA	2453	N.	THR	349		-31.784	37.764	1.00	0.00	. 3A7
ATOM	2454	CA	THR	349		-30.615 -29.394	37.512 38.153	1.00	0.00	3A7 3A7
ATOM ATOM	2455 2456	CB OG1	THR	349 349		-29.682	39.512	1.00	0.00	3A7
ATOM	2457		THR	349		-28.168	38.103	1.00	0.00	3A7
ATOM	2458	C	THR	349		-30.355	36.030	1.00	0.00	3A7
MOTA	2459	0	THR	349	6.224	-29.855	35.582	1.00	0.00	3A7
ATOM	2460	N	VAL	350		-30.735	35.203	1.00	0.00	3A7
ATOM	2461	CA	VAL	350		-30.585 -31.111	33.760 33.245	1.00	0.00	3A7 3A7
ATOM ATOM	2462 2463	CB CG1	VAL	350 350		-31.111	31.710	1.00	0.00	3A7
ATOM	2464		VAL	350		-30.188	33.784	1.00	0.00	3A7
ATOM	2465	c	VAL	350		-31.305	33.054	1.00	0.00	3A7
ATOM	2466	0	VAL	350	6.691	-30.900	31.980	1.00	0.00	3A7
ATOM	2467	N	LEU	351		-32.397	33.667	1.00	0.00	3A7
ATOM	2468	CA	LEU	351		-33.220	33.098	1.00	0.00	3A7
ATOM	2469 2470	CB	LEU	351 351		-34.682 -35.324	33.599 33.359	1.00	0.00	3A7 3A7
ATOM ATOM	2470	CG CD1	LEU	351		-36.712	34.024	1.00	0.00	3A7
ATOM	2472		LEU	351		-35.402	31.865	1.00	0.00	3A7
ATOM	2473	C	LEU	351	4.203	-32.710	33.432	1.00	0.00	3A7
ATOM	2474	0	LEU	351		-32.996	32.716	1.00	0.00	3A7
ATOM	2475	N	GLN	352		-31.949	34.546	1.00	0.00	3A7 3A7
ATOM	2476	CA	GLN	352	2.115	-31.491	35.037	1.00	0.00	JA /

ATOM	2477	СВ	GLN	352	2.625	-31.677	36.565	1.00	0.00	3A7
MOTA	2478	CG	GLN	352	2.109	-33.072	36.977	1.00	0.00	3A7
ATOM	2479	CD	GLN	352	3.125	-34.176	36.678	1.00	0.00	3A7
ATOM	2480		GLN	352	2.971	-34.938	35.716	1.00	0.00	3A7
ATOM	2481		GLN	352		-34.268	37.551	1.00	0.00	3A7
ATOM	2482	Ç	GLN	352		-30.043	34.711	1.00	0.00	3A7
ATOM	2483	ŏ	GLN	352		-29.394	35.333	1.00	0.00	3A7
						-29.394	33.712	1.00	0.00	3A7
MOTA	2484	N	LEU	353				1.00	0.00	3A7
ATOM	2485	CA	LEU	353		-28.104	33.338		0.00	3A7 3A7
ATOM	2486	CB	LEU	353		-27.396	33.371	1.00		
MOTA	2487	CG	LEU	353 .		-27.076	34.789	1.00	0.00	3A7
MOTA	2488		LEU	353		-26.787	34.712	1.00	0.00	3A7
MOTA	2489	CD2	LEU	353		-25.911	35.433	1.00	0.00	3A7
MOTA	2490	С	LEU	353	2.588	-28.000	31.951	1.00	0.00	3A7
ATOM	2491	0	LEU	353	3.198	-27.396	31.071	1.00	0.00	3A7
ATOM	2492	N	GLU	354	1.380	-28.556	31.747	1.00	0.00	3A7
ATOM	2493	CA	GLU	354	0.702	-28.679	30.481	1.00	0.00	3A7
ATOM	2494	СВ	GLU	354	-0.697	-29.284	30.692	1.00	0.00	3A7
ATOM	2495	CG	GLU	354		-30.790	31.013	1.00	0.00	3A7
ATOM	2496	CD	GLU	354		-31.081	32.431	1.00	0.00	3A7
ATOM	2497		GLU	354		-31.962	32.579	1.00	0.00	3A7
ATOM	2498		GLU	354		-30.446	33.382	1.00	0.00	3A7
ATOM	2499			354		-27.384	29.710	1.00	0.00	3A7
		C	GLU				28.531	1.00	0.00	3A7
MOTA	2500	0	GLU	354		-27.315				
ATOM	2501	N	TYR	355		-26.319	30.358	1.00	0.00	3A7
ATOM	2502	CA	TYR	355		-25.056	29.708	1.00	0.00	3A7
ATOM	2503	СВ	TYR	355		-24.126	30.584	1.00	0.00	3A7
MOTA	2504	CG	TYR	355		-24.797	30.922	1.00	0.00	. 3A7
MOTA	2505		TYR	355		-24.843	32.245	1.00	0.00	3A7
MOTA	2506	CD2	TYR	355		-25.427	29.938	1.00	0.00	3A7
ATOM	2507		TYR	355	-4.029	-25.504	32.585	1.00	0.00	3A7
ATOM	2508	CE2	TYR	355	-4.354	-26.101	30.275	1.00	0.00	3A7
MOTA	2509	CZ	TYR	355	-4.779	-26.138	31.599	1.00	0.00	3A7
MOTA	2510	OH	TYR	355	-5.972	-26.813	31.940	1.00	0.00	3A7
ATOM	2511	С	TYR	355	1.014	-24.314	29.358	1.00	0.00	3A7
ATOM	2512	0	TYR	355		-23.672	28.320	1.00	0.00	3A7
ATOM	2513	N	LEU	356		-24.432	30.194	1.00	0.00	3A7
ATOM	2514	CA	LEU	356		-23.853	29.929	1.00	0.00	3A7
ATOM	2515	СВ	LEU	356		-24.000	31.136	1.00	0.00	3A7
ATOM	2516	CG	LEU	356		-22.859	31.211	1.00	0.00	3A7
ATOM	2517		LEU	356		-22.429	32.674	1.00	0.00	3A7
ATOM	2518					-23.187		1.00	0.00	3A7
			LEU	356			30.588			
ATOM	2519	C	LEU	356		-24.430	28.735	1.00	0.00	3A7
ATOM	2520	0	LEU	356		-23.709	27.891	1.00	0.00	3A7
ATOM	2521	N	ASP	357		-25.778	28.619	1.00	0.00	3A7
MOTA	2522	CA	ASP	·357		-26.516	27.513	1.00	0.00	3A7
ATOM	2523	CB	ASP	357		-28.050	27.598	1.00	0.00	3A7
MOTA	2524	CG	ASP	357		-28.771	28.597	1.00	0.00	3A7
ATOM	.2525		ASP	357	5.958	-29.726	28.159	1.00	0.00	3A7
ATOM	2526	OD2	ASP	357	5.258	-28.397	29.796	1.00	0.00	3A7
ATOM	2527	С	ASP	357	4.055	-26.136	26.182	1.00	0.00	3A7
ATOM	2528	0	ASP	357	4.748	-25.985	25.183	1.00	0.00	3A7
ATOM	2529	N	MET	358	2.719	-25.956	26.163	1.00	0.00	3A7
ATOM	2530	CA	MET	358	1.969	-25.573	24.997	1.00	0.00	3A7
ATOM	2531	СВ	MET	358		-25.711	25.263	1.00	0.00	3A7
ATOM	2532	CG	MET	358		-27.178	25.430	1.00	0.00	3A7
ATOM	2533	SD	MET	358		-27.420	26.341	1.00	0.00	3A7
ATOM	2534	CE	MET	358		-26.461	25.262	1.00	0.00	3A7
ATOM	2535	c	MET	358		-24.149	24.601	1.00	0.00	3A7
ATOM	2536	Ö	MET	358		-23.825	23.421	1.00	0.00	3A7
ATOM	2537		VAL	359		-23.255	25.594	1.00	0.00	3A7
		N								3A7 3A7
ATOM	2538	CA	VAL	359		-21.869	25.376	1.00	0.00	
ATOM	2539	CB	VAL	359		-21.083	26.684	1.00	0.00	3A7
MOTA	2540	CG1		359		-19.776	26.626	1.00	0.00	3A7
ATOM	2541	CG2		359		-20.783	27.005	1.00	0.00	3A7
MOTA	2542	С	VAL	359		-21.791	24.701	1.00	0.00	3A7
MOTA	2543	0	VAL	359		-21.063	23.725	1.00	0.00	3A7
MOTA	2544	N	VAL	360		-22.575	25.182	1.00	0.00	3A7
MOTA	2545	CA	VAL	360	6.556	-22.600	24.616	1.00	0.00	3A7
MOTA	2546	CB	VAL	360	7.506	-23.421	25.479	1.00	0.00	3A7
MOTA	2547	CG1		360		-23.573	24.831	1.00	0.00	3A7
ATOM	2548	CG2		360		-22.713	26.844	1.00	0.00	3A7

ATOM	2549	С	VAL	360	6.520	-23.153	23.207	1.00	0.00	3A7
ATOM	2550	ō	VAL	360		-22.609	22.323	1.00	0.00	3A7
			ASN	361		-24.208	22.949	1.00	0.00	3A7
ATOM	2551	N								
ATOM	2552	CA	ASN	361		-24.789	21.630	1.00	0.00	3A7
MOTA	2553	CB	ASN	361	4.650	-26.030	21.669	1.00	0.00	3A7
ATOM	2554	CG	ASN	361	5.417	-27.219	22.258	1.00	0.00	3A7
ATOM	2555		ASN	361		-27.329	22.121	1.00	0.00	3A7
MOTA	2556	ND2	ASN	361		-28.135	22.930	1.00	0.00	3A7
MOTA	2557	С	ASN	361	4.952	-23.808	20.655	1.00	0.00	3A7
ATOM	2558	0	ASN	361	5.410	-23.694	19.523	1.00	0.00	3A7
ATOM	2559	N	GLU	362		-23.044	21.087	1.00	0.00	3A7
										3A7
ATOM	2560	CA	GLU	362		-21.994	20.287	1.00	0.00	
ATOM	2561	CB	GLU	362	2.013	-21.499	20.896	1.00	0.00	3A7
ATOM	2562	CG	GLU	362	1.224	-20.515	20.011	1.00	0.00	3A7
ATOM	2563	CD	GLU	362	0.583	-21.183	18.798	1.00	0.00	3A7
				362		-22.314	18.429	1.00	0.00	3A7
ATOM	2564		GLU							
ATOM	2565	OE2	GLU	362		-20.534	18.190	1.00	0.00	3A7
ATOM	2566	С	GLU	362	4.241	-20.837	20.000	1.00	0.00	3A7
ATOM	2567	0	GLU	362	4.205	-20.266	18.913	1.00	0.00	3A7
ATOM	2568	N	THR	363		-20.478	20.946	1.00	0.00	3A7
										3A7
MOTA	2569	CA	THR	363		-19.416	20.720	1.00	0.00	
ATOM	2570	CB	THR	363	6.793	-19.002	21.991	1.00	0.00	3A7
ATOM	2571	OG1	THR	363	5.804	-18.623	22.938	1.00	0.00	3A7
ATOM	2572		THR	363		-17.778	21.706	1.00	0.00	3A7
							19.666	1.00	0.00	3A7
MOTA	2573	С	THR	363		-19.831				
MOTA	2574·	0	THR '	363		-19.042	18.805	1.00	0.00	3A7
ATOM	2575	N	LEU	364	7.504	-21.115	19.676	1.00	0.00	3A7
MOTA	2576	CA	LEU	364	8.417	-21.641	18.695	1.00	0.00	3A7
ATOM	2577	СВ	LEU	364		-23.014	19.086	1.00	0.00	3A7
							20.283	1.00	0.00	3A7
MOTA	2578	CG	LEU	364		-23.018				
ATOM	2579	CD1	LEU	364	10.242	-24.462	20.696	1.00	0.00	3A7
ATOM	2580	CD2	LEU	364	11.219	-22.259	19.974	1.00	0.00	3A7
MOTA	2581	С	LEU	364	7.769	-21.746	17.338	1.00	0.00	3A7
ATOM	2582	ŏ	LEU	364		-21.492	16.324	1.00	0.00	3A7
										3A7
MOTA	2583	И	ARG	365		-22.094	17.264	1.00	0.00	
MOTA	2584	CA	ARG	365	5.743	-22.109	16.003	1.00	0.00	. 3A7
MOTA	2585	CB	ARG	365	4.300	-22.612	16.169	1.00	0.00	3A7
ATOM	2586	CG	ARG	365	3.614	-22.980	14.858	1.00	0.00	3A7
ATOM	2587	CD	ARG	365		-23.285	15.005	1.00	0.00	3A7
									*	
MOTA	2588	NE	ARG	365		-21.987	15.068	1.00	0.00	3A7
MOTA	2589	CZ	ARG	365	0.011	-21.942	15.201	1.00	0.00	3A7
ATOM	2590	NHl	ARG	365	-0.637	-20.742	15.124	1.00	0.00	3A7
ATOM	2591	NH2	ARG	365	-0.703	-23.084	15.418	1.00	0.00	3A7
ATOM	2592	С	ARG	365		-20.756	15.371	1.00	0.00	3A7
										3A7 .
ATOM	2593	0	λRG	365		-20.573	14.192	1.00	0.00	
ATOM	2594	N	LEU	366	5.239	-19.760	16.176	1.00	0.00	3A7
ATOM	2595	CA	LEU	366	5.030	-18.410	15.729	1.00	0.00	3A7
MOTA	2596	CB	LEU	366	4.204	-17.608	16.752	1.00	0.00	3A7
ATOM	2597	CG	LEU	366		-16.833	16.122	1.00	0.00	3A7
-										
ATOM	2598		LEU	366		-16.361	17.201	1.00	0.00	3A7
ATOM	2599	CD2	LEU	366		-15.648	15.240	1.00	0.00	3A7
MOTA	2600	С	LEU	366	6.295	-17.670	15.380	1.00	0.00	3A7
ATOM	2601	0	LEU	366	6.339	-16.992	14.359	1.00	0.00	3A7
ATOM	2602	N	PHE	367		-17.798	16.193	1.00	0.00	3A7
									0.00	3A7
ATOM	2603	CA	PHE	367		-17.136	15.897	1.00		
ATOM	2604	СВ	PHE	367		~16.072	16.907	1.00	0.00	3A7
ATOM	2605	CG	PHE	367	7.886	-15.081	17.042	1.00	0.00	3A7
MOTA	2606	CD1		367		-15.250	18.035	1.00	0.00	3A7
ATOM	2607		PHE	367		-13.998	16.170	1.00	0.00	3A7
							18.137	1.00	0.00	3A7
ATOM	2608		PHE	367		-14.365				
ATOM	2609		PHE	367		-13.100	16.285	1.00	0.00	3A7
ATOM	2610	CZ	PHE	367	5.757	-13.284	17.269	1.00	0.00	3A7
ATOM	2611	С	PHE	367	9.740	-18.121	15.878	1.00	0.00	3A7
MOTA	2612	ō	PHE	367		-18.207	16.823	1.00	0.00	3A7
						-18.877				3A7
ATOM	2613	N	PRO	368			14.814	1.00	0.00	
MOTA	2614	CA	PRO	368		-19.868	14.730	1.00	0.00	3A7
ATOM	2615	CD	PRO	368	8.891	-19.039	13.788	1.00	0.00	3A7
ATOM	2616	СВ	PRO	368	10.570	-20.710	13.544	1.00	0.00	3A7
ATOM	2617	CG	PRO	368		-19.942	12.757	1.00	0.00	3A7
							14.589	1.00		3A7
ATOM	2618	С	PRO	368		-19.200			0.00	
MOTA	2619	0	PRO	368		-18.434	13.657	1.00	0.00	3A7
ATOM	2620	N	VAL	369	13.143	-19.481	15.561	1.00	0.00	3A7
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ATOM	2621	CA	VAL	369	14.427	-18.858	15.709	1.00	0.00	3A7
MOTA	2622	СВ	VAL	369		-19.329	16.991	1.00	0.00	3A7
ATOM	2623		VAL	369		-18.705	17.115	1.00	0.00	3A7 3A7
MOTA	2624 2625	CGZ	VAL VAL	369 369		-18.876 -19.141	18.133 14.529	1.00	0.00	3A7
ATOM ATOM	2625	Ö	VAL	369		-18.284	14.109	1.00	0.00	3A7
ATOM	2627	N	ALA	370		-20.349	13.946	1.00	0.00	3A7
ATOM	2628	CA	ALA	370		-20.686	12.775	1.00	0.00	, 3A7
ATOM	2629	СВ	ALA	370	16.677	-22.035	12.966	1.00	0.00	3A7
MOTA	2630	С	ALA	370		-20.739	11.619	1.00	0.00	3A7
ATOM	2631	0	ALA	370		-21.792 -19.597	11.309 10.938	1.00 1.00	0.00 0.00	3A7 3A7
ATOM ATOM	2632 2633	N CA	MET MET	371 371		-19.337	9.924	1.00	0.00	3A7
ATOM	2634	СВ	MET	371		-17.940	9.616	1.00	0.00	3A7
ATOM	2635	CG	MET	371		-17.053	9.800	1.00	0.00	3A7
ATOM	2636	SD	MET	371		-17.276	8.566	1.00	0.00	3A7
ATOM	2637	CE	MET	371		-16.484	7.182	1.00	0.00	3A7 3A7
ATOM	2638	C	MET MET	371 371		-20.142 -20.260	8.625 7.783	1.00 1.00	0.00	3A7
ATOM ATOM	2639 2640	0 N	ARG	372		-20.200	8.432	1.00	0.00	3A7
ATOM	2641	CA	ARG	372		-21.368	7.254	1.00	0.00	3A7
ATOM	2642	СВ	ARG	372		-20.480	6.088	1.00	0.00	3A7
ATOM	2643	CG	ARG	372		-19.769	5.248	1.00	0.00	3A7
ATOM	2644	CD	ARG	372		-19.020	4.096	1.00	0.00	3A7 3A7
ATOM	2645	NE	ARG	372 372		-18.673 -19.599	2.996 2.066	1.00	0.00	3A7
ATOM ATOM	2646 2647	CZ NH1	ARG ARG	372		-19.194	0.870	1.00	0.00	3A7
ATOM	2648		ARG	372		-20.930	2.301	1.00	0.00	3A7
ATOM	2649	¢	ARG	372		-22.309	7.639	1.00	0.00	3A7
ATOM	2650	0	ARG	372		-22.029	8.542	1.00	0.00	3A7
MOTA	2651	N	LEU	373		-23.453	6.907	1.00	0.00	3A7 3A7
MOTA	2652	CA CB	LEU	373 373		-24.462 -25.879	7.034 7.360	1.00	0.00	3A7
ATOM ATOM	2653 2654	CG	LEU	373		-26.016	8.700	1.00	0.00	3A7
ATOM	2655		LEU			-25.305	9.860	1.00	0.00	3A7
ATOM	2656	CD2	LEU	373	15.150	-25.605	8.611	1.00	0.00	3A7
MOTA	2657	С	LEU	373		-24.532	5.697	1.00	0.00	3A7
ATOM	2658	0	LEU	373		-23.979	4.717	1.00 1.00	0.00	3A7 · 3A7
ATOM ATOM	2659 2660	N CA	GLU GLU	374 374		-25.232 -25.477	5.619 4.356	1.00	0.00	3A7
ATOM	2661	СВ	GLU	374		-24.637	4.153	1.00	0.00	3A7
ATOM	2662	CG	GLU	374		-23.121	4.279	1.00	0.00	3A7
ATOM	2663	CD	GLU	374		-22.422	4.038	1.00	0.00	3A7
ATOM	2664		GLU	374		-21.801	5.000	1.00	0.00	3A7 3A7
ATOM	2665		GLU	374 374		-22.501 -26.936	2.889 4.222	1.00	0.00	3A7
ATOM ATOM	2666 2667	С О	GLU GLU	374		-27.553	5.141	1.00	0.00	3A7
ATOM	2668	N	ARG	375		-27.510	3.026	1.00	0.00	3A7
MOTA	2669	CA	ARG	. 375	20.879	-28.878	2.666	1.00	0.00	3A7
ATOM	2670	CB	ARG	375		-29.770	2.636	1.00	0.00	3A7
MOTA	2671	CG	ARG	375		-30.018	4.037	1.00	0.00	3A7 3A7
MOTA MOTA	2672 2673	CD NE	ARG ARG	· 375 375		-30.919 -31.381	5.436	1.00 1.00	0.00	3A7
ATOM	2674	CZ	ARG	375		-30.590	6.396		0.00	3A7
ATOM	2675	NH1	ARG	375	16.734	-31.096	7.650	1.00	0.00	3A7
ATOM	2676	NH2	ARG	375		-29.307	6.125	1.00	0.00	3A7
MOTA	2677	C	ARG	375		-28.826	1.293	1.00	0.00	3A7
ATOM	2678	0	ARG .	375 376		-27.846 -29.890	0.569 0.889	1.00	0.00	3A7 3A7
MOTA MOTA	2679 2680	N CA	VAL VAL	376		-29.949	-0.420	1.00	0.00	3A7
ATOM	2681	СВ	VAL	376		-29.725	-0.397	1.00	0.00	3A7
MOTA	2682	CG1	VAL	376	24.936	-29.796	-1.822	1.00	0.00	3A7
MOTA	2683		VAL	376		-28.346	0.234	1.00	0.00	3A7
ATOM	2684	C	VAL	376 376		-31.316	-0.934	1.00	0.00	3A7 3A7
ATOM ATOM	2685 2686	о И	VAL CYS	376 377		-32.316 -31.397	-0.233 -2.212	1.00	0.00	3A7
ATOM	2687	CA	CYS	377		-32.642	-2.851	1.00	0.00	3A7
ATOM	2688	СВ	CYS	377		-32.435	-4.083	1.00	0.00	3A7
ATOM	2689	SG	CYS	377		-31.876	-3.569	1.00	0.00	3A7
ATOM	2690	C	CYS	377		-33.392	-3.254	1.00	0.00	3A7
MOTA	2691	0	CYS	377		-32.843	-3.794	1.00	0.00	3A7 3A7
ATOM	2692	N	LYS	378	44.904	-34.705	-2.955	1.00	0.00	JAI

MOTA	2693	CA	LYS	378	24.083	-35.594	-3.143	1.00	0.00	3A7
ATOM	2694	СВ	LYS	378		-36.718	-2.075	1.00	0.00	3A7
MOTA	2695	CG	LYS	378		-36.428	-0.894	1.00	0.00	3A7
ATOM	2696	CD	LYS	378		-37.592	0.101	1.00	0.00	3A7 3A7
MOTA MOTA	2697 2698	CE NZ	LYS LYS	378 378		-37.375 -36.159	1.174	1.00	0.00	3A7
ATOM	2699	C	LYS	378		-36.202	-4.524	1.00	0.00	3A7
ATOM	2700	ŏ	LYS	378		-36.609	-5.075	1.00	0.00	3A7
ATOM	2701	N	LYS	379		-36.285	-5.081	1.00	0.00	3A7
ATOM	2702	CA	LYS	379		-36.939	-6.329	1.00	0.00	3A7
MOTA	2703	СB	LYS	379		-38.417	-6.127	1.00	0.00	3A7
ATOM	2704	CG	LYS	379		-38.609	-5.161	1.00	0.00	3A7
ATOM	2705 2706	CD	LYS	379 379		-40.083 -40.842	-4.899 -4.120	1.00	0.00	3A7 3A7
ATOM ATOM	2707	CE NZ	LYS	379		-42.233	-3.850	1.00	0.00	3A7
ATOM	2708	c	LYS	379		-36.155	-6.981	1.00	0.00	3A7
ATOM	2709	0	LYS	379		-35.119	-6.483	1.00	0.00	3A7
ATOM	2710	N	ASP	380		-36.650	-8.134	1.00	0.00	3A7
ATOM	2711	CA	ASP	380		-36.071	-8.818	1.00	0.00	3A7
ATOM	2712	СВ	ASP	380		-36.404		1.00	0.00	3A7
ATOM	2713	CG	ASP	380		-35.921 -34.689		1.00	0.00	3A7 3A7
ATOM ATOM	2714 2715		ASP ASP	380 380		-36.782		1.00	0.00	3A7
ATOM	2716	C	ASP	380		-36.616	-8.182	1.00	0.00	3A7
ATOM	2717	ō	ASP	380		-37.798	-7.848	1.00	0.00	3A7
MOTA	2718	N	VAL	381	17.554	-35.744	-7.966	1.00	0.00	3A7
MOTA	2719	CA	VAL	381		-36.118	-7.224	1.00	0.00	3A7
ATOM	2720	СВ	VAL	381		-35.910	-5.720	1.00	0.00	3A7
ATOM ATOM	2721 2722		VAL	381 381		-34.439 -36.489	-5.360 -4.947	1.00	0.00	3A7 3A7
MOTA	2723	C	VAL	381		-35.308	-7.781	1.00	0.00	3A7
ATOM	2724	ŏ	VAL	381		-34.151	-8.142	1.00	0.00	3A7
ATOM	2725	N	GLU	382	14.045	-35.908	-7.874	1.00	0.00	3A7
ATOM	2726	CA	GLU	382		-35.247	-8.420	1.00	0.00	3A7
MOTA	2727	СВ	GLU	382		-36.100	-9.485	1.00	0.00	3A7
ATOM	2728	CG	GLU	382		-36.325		1.00	0.00	3A7 3A7
ATOM ATOM	2729 2730	CD OE1	GLU GLU	382 382		-37.311 -38.470		1.00	0.00	3A7
ATOM	2731		GLU	382			-10.822	1.00	0.00	3A7
MOTA	2732	С	GLU	382	11.952	-34.980	-7.271	1.00	0.00	3A7
ATOM	2733	0	GLU	382		-35.909	-6.587	1.00	0.00	3A7
ATOM	2734	N	ILE	383		-33.690	-7.028	1.00	0.00	3A7
ATOM ATOM	2735 ⁻ 2736	CA CB	ILE	383 383		-33.270 -32.299	-5.937 -4.973	1.00	0.00	3A7 3A 7
MOTA	2737		ILE	383		-32.043	-3.747	1.00	0.00	3A7
ATOM	2738		ILE	383		-32.774	-4.555	1.00	0.00	3A7
MOTA	2739	CD	ILE	383	12.883	-34.026	-3.677	1.00	0.00	3A7
ATOM	2740	С	ILE	383		-32.594	-6.567	1.00	0.00	3A7
MOTA	2741	0.	ILE	383		-31.493	-7.103	1.00	0.00	. 3A7
ATOM ATOM	2742 2743	N CA	ASN ASN	384 384		-33.254 -32.719	-6.521 -6.976	1.00	0.00	3A7 . 3A7
ATOM	2744	CB	ASN	384		-31.411	-6.222	1.00	0.00	3A7
ATOM	2745	CG	ASN	384		-31.147	-6.283	1.00	0.00	3A7
ATOM	2746		ASN	384		-30.251	-7.000	1.00	0.00	3A7
MOTA	2747		ASN	384		-31.956	-5.498	1.00	0.00	3A7
ATOM	2748	C	ASN	384		-32.504		1.00	0.00	3A7
ATOM ATOM	2749 2750	O N	ASN GLY	384 385		-31.623 -33.322	-8.988 -9.231	1.00	0.00	3A7 3A7
ATOM	2751	CA	GLY	385		-33.246		1.00	0.00	3A7
ATOM	2752	c	GLY	385		-32.342		1.00	0.00	3A7
MOTA	2753	0	GLY	385	9.217	-32.266	-12.366	1.00	0.00	3A7
MOTA	2754	N	MET	386		-31.631		1.00	0.00	3A7
ATOM	2755	CA	MET	386		-30.773		1.00	0.00	3A7
ATOM	2756	CB	MET	386 386		-29.264		1.00	0.00	3A7 3A7
MOTA MOTA	2757 2758	CG SD	MET MET	386 386		-28.845 -27.091	-8.990 -8.895	1.00	0.00	3A7 3A7
ATOM	2759	CE	MET	386		-26.373		1.00	0.00	3A7
ATOM	2760	c	MET	386		-31.305		1.00	0.00	3A7
MOTA	2761	0	MET	386		-31.654	-9.025	1.00	0.00	3A7
ATOM	2762	N	PHE	387		-31.396		1.00	0.00	3A7
ATOM	2763	CA	PHE	387		-32.074		1.00	0.00	3A7
MOTA	2764	СВ	PHE	387	14.935	-32.474	-12.3/8	1.00	0.00	3A7

ATOM	2765	CG	PHE	387	14.102	-33.505	-13.091	1.00	0.00	3A7
ATOM	2766		PHE	387		-34.767		1.00	0.00	3A7
			PHE	387		-33.213		1.00	0.00	3A7
ATOM	2767							1.00	0.00	3A7
ATOM	2768		PHE	387		-35.727				
ATOM	2769		PHE	387		-34.173		1.00	0.00	3A7
ATOM	2770	CZ	PHE	387	12.642	-35.433	-14.507	1.00	0.00	3A7
ATOM	2771	С	PHE	387	15.405	-31.180	-10.312	1.00	0.00	3A7
ATOM	2772	0	PHE	387		-30.043		1.00	0.00	3A7
	_	N	ILE	388		-31.706	-9.251	1.00	0.00	3A7
ATOM	2773							1.00	0.00	3A7
ATOM	2774	CA	ILE	388		-31.049	-8.544			
MOTA	2775	СВ	ILE	388		-31.071	-7.032	1.00	0.00	3A7
ATOM	2776	CG2	ILE	388	18.144	-30.276	-6.387	1.00	0.00	3A7
ATOM	2777	ÇG1	ILE	388	15.641	-30.487	-6.591	1.00	0.00	3A7
ATOM	2778	CD	ILE	388	15.434	-29.010	-6.913	1.00	0.00	3A7
ATOM	2779	С	ILE	388		-31.746	-8.935	1.00	0.00	3A7
	2780	ŏ	ILE	388		-32.952	-8.728	1.00	0.00	3A7
ATOM							-9.496	1.00	0.00	3A7
ATOM	2781	N	PRO	389		-31.021				
ATOM	2782	CA	PRO	389 .		-31.581	-9.867	1.00	0.00	3A7
MOTA	2783	CD	PRO	389	19.063	-29.901	-10.375	1.00	0.00	3A7
ATOM	2784	CB	PRO	389	21.290	-30.549	-10.822	1.00	0.00	3A7
ATOM	2785	CG	PRO	389	20.081	-29.931	-11.509	1.00	0.00	3A7
ATOM	2786	c	PRO ·	389		-31.785	-8.684	1.00	0.00	3A7
						-31.121	-7.659	1.00	0.00	3A7
ATOM	2787	0	PRO	389					0.00	3A7
ATOM	2788	N	LYS	390		-32.663	-8.836	1.00		
ATOM	2789	CA	LYS	390	23.654	-32.884	-7.847	1.00	0.00	3A7
ATOM	2790	ÇВ	LYS	390	24.733	-33.851	-8.363	1.00	0.00	3A7
ATOM	2791	CG	LYS	390	24.234	-35.053	-9.176	1.00	0.00	3A7
ATOM	2792	CD	LYS	390		-36.029	-9.517	1.00	0.00	3A7
				390		-37.258		1.00	0.00	3A7
MOTA	2793	CE	LYS				-9.538	1.00	0.00	3A7
MOTA	2794	NZ	LYS	390		-38.073				
ATOM	2795	С	LYS	390		-31.584	-7.486	1.00	0.00	3A7
ATOM	2796	0	LYS	390	24.631	-30.776	-8.366	1.00	0.00	3A7
MOTA	2797	N	GLY	391	24.558	-31.329	-6.177	1.00	0.00	3A7
ATOM	2798	CA	GLY	391	25.250	-30.153	-5.707	1.00	0.00	3A7
ATOM	2799	C	GLY	391		-28.926	-5.567	1.00	0.00	3A7
ATOM	2800	ŏ	GLY	391		-27.848	-5.320	1.00	0.00	3A7
						-29.029	-5.690	1.00	0.00	3A7
ATOM	2801	N	VAL	392					0.00	3A7
ATOM	2802	CA	VAL	392		-27.896	-5.522	1.00		
ATOM	2803	СB	VAL	392		-28.126	-6.224	1.00	0.00	3A7
ATOM	2804	CG1	VAL	392	19.765	-27.062	-5.883	1.00	0.00	3A7
ATOM	2805	CG2	VAL	392	21.074	-28.134	-7.744	1.00	0.00	3A7
ATOM	2806	С	VAL	392	21.922	-27.684	-4.050	1.00	0.00	3A7
ATOM	2807	ō	VAL	392		-28.644	-3.290	1.00	0.00	3A7
				393		-26.403	-3.629	1.00	0.00	3A7
ATOM	2808	N	VAL							3A7
MOTA	2809	CA	VAL	393		-26.024	-2.268	1.00	0.00	
ATOM	2810	CB	VAL	393		-24.695	-1.900	1.00	0.00	3A7
ATOM	2811	CG1	VAL	393	21.828	-24.336	-0.425	1.00	0.00	3A7
ATOM	2812	CG2	VAL	393	23.636	-24.785	-2.160	1.00	0.00	3A7
ATOM	2813	С	VAL	393	19.992	-25.964	-2.130	1.00	0.00	3A7
ATOM	2814	ō	VAL	393		-25.288	-2.891	1.00	0.00	3A7
		N		394		-26.712	-1.145	1.00	0.00	3A7
ATOM	2815		VAL					1.00	0.00	3A7
ATOM	2816	CA	VAL	394		-26.825	-0.864			
ATOM	2817	СВ	VAL	394		-28.282	-0.810	1.00	0.00	3A7
ATOM	2818	CG1	VAL	394		-28.411	-0.510	1.00	0.00	3A7
ATOM	2819	CG2	VAL	394	17.948	-28.936	-2.163	1.00	0.00	3A7
ATOM	2820	C	VAL	394		-26.177	0.471	1.00	0.00	3A 7
ATOM	2821	ŏ	VAL	394		-26.423	1.400	1.00	0.00	3A7
				395		-25.325	0.609	1.00	0.00	3A7
ATOM	2822	N	MET							3A7
MOTA	2823	CA	MET	395		-24.656		1.00	0.00	
ATOM	2824	CB	MET		16.818		1.809	1.00	0.00	3A7
ATOM	2825	CG	MET	395		-22.812	1.578	1.00	0.00	3A7
MOTA	2826	SD	MET	395	18.747	-21.101	2.015	1.00	0.00	3A7
ATOM	2827	CE	MET	395	17.770	-20.277	0.725	1.00	0.00	3A7
ATOM	2828	c	MET	395		-24.885		1.00	0.00	3A7
						-24.925		1.00	0.00	3A7
ATOM	2829	0	MET	395					0.00	3A7
ATOM	2830	N	ILE	396		-25.076		1.00		
ATOM	2831	CA	ILE	396		-25.356		1.00	0.00	3A7
MOTA	2832	CB	ILE	396	13.599	-26.610		1.00	0.00	3A7
ATOM	2833	CG2		396	12.490	-26.667	5.983	1.00	0.00	3A7
ATOM	2834			396		-27.897		1.00	0.00	3A7
ATOM	2835	CD	ILE	396		-28.104		1.00	0.00	3A7
						-24.182		1.00	0.00	3A7
ATOM	2836	С	ILE	396	17.100	-24.102	7.302	1.00	5.05	

ATOM	2837	0	ILE	396	13.874	-23.964	5.894	1.00	0.00	3A7
ATOM	2838	N	PRO	397		-23.398	4.590	1.00	0.00	3A7
ATOM	2839	CA	PRO	397		-22.297	5.462	1.00	0.00	3A7
ATOM	2840	CD	PRO	397		-23.022	3.209	1.00	0.00	3A7 3A7
MOTA	2841	CB CG	PRO	397 397		-21.252 -22.043	4.533 3.293	1.00	0.00	3A7
MOTA ATOM	2842 2843	C	PRO	397		-22.717	6.544	1.00	0.00	3A7
ATOM	2844	ō	PRO	397		-22.732	6.310	1.00	0.00	3A7
ATOM	2845	N	SER	398		-22.981	7.767	1.00	0.00	3A7
ATOM	2846	CA	SER	398	10.575	-23.392	8.914	1.00	0.00	3A7
ATOM	2847	CB	SER	398		-23.676	10.138	1.00	0.00	3A7
MOTA	2848	OG	SER	398		-22.517	10.613	1.00	0.00	3A7
ATOM	2849	С	SER	398		-22.379	9.316	1.00	0.00	3A7
ATOM	2850	0	SER	398 399		-22.745 -21.053	9.668 9.231	1.00	0.00	3A7 3A7
ATOM ATOM	2851 2852	N CA	TYR TYR	399		-19.958	9.507	1.00	0.00	3A7
ATOM	2853	СВ	TYR	399		-18.562	9.264	1.00	0.00	3A7
ATOM	2854	CG	TYR	399	9.084	-17.492	10.212	1.00	0.00	3A7
ATOM	2855	CD1	TYR	399	9.933	-16.936	11.172	1.00	0.00	3A7
ATOM	2856		TYR	399		-17.008	10.123	1.00	0.00	3A7
ATOM	2857		TYR	399		-15.959	12.051	1.00	0.00	3A7
ATOM	2858		TYR	399		-16.041 -15.520	11.007	1.00	0.00	3A7 3A 7
MOTA ATOM	2859 2860	CZ OH	TYR TYR	399 399		-14.553	12.880	1.00	0.00	3A7
ATOM	2861	C	TYR	399		-20.038	8.647	1.00	0.00	3A7
ATOM	2862	ŏ	TYR	399		-19.765	9.067	1.00	0.00	3A7
MOTA	2863	N	VAL	400	7.911	-20.472	7.398	1.00	0.00	3A7
ATOM	2864	CA	VAL	400		-20.616	6.436	1.00	0.00	3A7
ATOM	2865	CB	VAL	400		-20.658	5.045	1.00	0.00	. 3A7
MOTA	2866		VAL	400		-20.758	4.020 4.899	1.00	0.00	3A7 3A7
MOTA MOTA	2867 2868	C	VAL VAL	400 400		-19.308 -21.827	6.653	1.00	0.00	3A7
ATOM	2869	o	VAL	400		-21.734	6.547	1.00	0.00	3A7
ATOM	2870	N	LEU	401		-22.992	6.970	1.00	0.00	3A7
ATOM	2871	CA	LEU	401	5.875	-24.224	7.175	1.00	0.00	3A7
MOTA	2872	CB	LEU	401		-25.449	7.318	1.00	0.00	3A7
ATOM	2873	CG	LEU	401		-25.453	6.535	1.00	0.00	3A7
ATOM	2874		LEU	401		-26.722 -25.294	6.915 5.023	1.00	0.00	3A7 3A7
MOTA MOTA	2875 2876	CD2	LEU	401 401		-24.186	8.449	1.00	0.00	3A7
ATOM	2877	ŏ	LEU	401		-24.705	8.504	1.00	0.00	3A7
ATOM	2878	N	HIS	402		-23.512	9.509	1.00	0.00	3A7
ATOM .	2879	CA	HIS	402		-23.303	10.782	1.00	0.00	3A7
ATOM	2880		HIS	402		-24.809	12.042	1.00	0.00	3A7
ATOM	2881	CG	HIS HIS	402		-23.553 -22.628	12.480 11.778	1.00	0.00	3A7 3A7
ATOM ATOM	2882 2883	CB	HIS	402 402		-24.122	13.375	1.00	0.00	3A7
MOTA	2884		HIS	402		-23.155	13.305	1.00	0.00	3A7
ATOM	2885		HIS	402		-25.085	12.595	1.00	0.00	3A7
ATOM	2886	С	HIS	402	3.648	-22.420	10.674	1.00	0.00	3A7
MOTA	2887	0	HIS	402		-22.343	11.602	1.00	0.00	3A7
ATOM	2888	N	HIS	403		-21.730 -20.839	9.522	1.00	0.00	3A7 3A7
ATOM ATOM	2889 2890	CA ND1	HIS HIS	403 403		-19.115	9.280 10.966	1.00	0.00	3A7
ATOM	2891	CG	HIS	403		-18.746	10.299	1.00	0.00	3A7
ATOM	2892	СВ	HIS	403		-19.394	9.048	1.00	0.00	3A7
ATOM	2893	NE2	HIS	403		-17.451	12.131	1.00	0.00	3A7
MOTA	2894		HIS	403		-17.730	11.028	1.00	0.00	3A7
ATOM	2895		HIS	403		-18.308	12.051	1.00	0.00	3A7 3A7
ATOM	2896	C	HIS	403 403		-21.280 -20.492	8.096 7.500	1.00	0.00	3A7
ATOM ATOM	2897 2898	о и	HIS ASP	404		-22.588	7.740	1.00	0.00	3A7
ATOM	2899	CA	ASP	404		-23.143	6.662	1.00	0.00	3A7
ATOM	2900	СВ	ASP	404		-24.585	6.322	1.00	0.00	3A7
MOTA	2901	CG	ASP	404		-25.218	5.103	1.00	0.00	3A7
MOTA	2902		ASP	404		-24.540	4.402	1.00	0.00	3A7
ATOM	2903		ASP	404		-26.417	4.850	1.00	0.00	3A7
ATOM	2904	C	ASP	404		-23.164 -23.809	7.105 8.108	1.00	0.00	3A7 3A7
ATOM ATOM	2905 2906	O N	ASP PRO	404 405		-23.809	6.421	1.00	0.00	3A7
ATOM	2907	CA	PRO	405		-22.344	6.827	1.00	0.00	3A7
ATOM	2908	CD	PRO	405		-21.674	5.237	1.00	0.00	3A7
		-								

ATOM	2909	СВ	PRO	405	-3.543	-21.309	5.854	1.00	0.00	3A7
	2910			405			4.621	1.00	0.00	3A7
MOTA		CG	PRO			-21.373				
ATOM	2911	С	PRO	405		-23.646	6.756	1.00	0.00	3A7
ATOM	2912	0	PRO	405	-4.766	-23.734	7.420	1.00	0.00	3A7
MOTA	2913	N	LYS	406	-3.297	-24.674	5.989	1.00	0.00	3A7
MOTA	2914	CA	LYS	406		-25.942	5.892	1.00	0.00	. 3A7
								1.00	0.00	3A7
ATOM	2915	CB	LYS	406		-26.748	4.646			
ATOM	2916	CG	LYS	406	-3.805	-26.004	3.326	1.00	0.00	3A7
ATOM	2917	CD	LYS	406	-3.234	-26.692	2.072	1.00	0.00	3A7
ATOM	2918	CE	LYS	406	-3.939	-27.993	1.650	1.00	0.00	3A7
ATOM	2919	NZ	LYS	406		-29.127	2.541	1.00	0.00	3A7
ATOM	2920	С	LYS	406		-26.791	7.115	1.00	0.00	3A7
ATOM	2921	0	LYS	406	-4.554	-27.622	7.479	1.00	0.00	3A7
ATOM	2922	N	TYR	407	-2.572	-26.584	7.783	1.00	0.00	3A7
ATOM	2923	CA	TYR	407	-2.174	-27.340	8.948	1.00	0.00	3A7
	2924			407		-27.703	8.898	1.00	0.00	3A7
ATOM		СВ	TYR							
MOTA	2925	CG	TYR	407		-28.906	8.000	1.00	0.00	3A7
ATOM	2926	CD1	TYR	407	-0.674	-28.783	6.613	1.00	0.00	3A7
ATOM	2927	CD2	TYR	407	-0.492	-30.184	8.557	1.00	0.00	3A7
ATOM	2928		TYR	407	-0.693	-29.912	5.799	1.00	0.00	3A7
						-31.314	7.746	1.00	0.00	3A7
ATOM	2929		TYR	407	•					
ATOM	2930	CZ	TYR	407		-31.179	6.365	1.00	0.00	3A7
ATOM	2931	OH	TYR	407	-0.583	-32.324	5.538	1.00	0.00	3A7
ATOM	2932	С	TYR	407	-2.474	-26.584	10.218	1.00	0.00	3A7
ATOM	2933	0	TYR	407		-27.189	11.229	1.00	0.00	3A7
		-							0.00	3A7
ATOM	2934	N	TRP	408		-25.240	10.202	1.00		
MOTA	2935	CA	TRP	408	-2.553	-24.414	11.368	1.00	0.00	3A7
ATOM	2936	CB	TRP	408	-1.243	-23.786	11.891	1.00	0.00	3A7
ATOM	2937	CG	TRP	408	-0.242	-24.837	12.291	1.00	0.00	3A7
ATOM	2938		TRP	408		-25.818	13.304	1.00	0.00	3A7
										3A7
ATOM	2939		TRP	408		-25.107	11.823	1.00	0.00	
ATOM	2940	NEI	TRP	· 408		-26.195	12.482	1.00	0.00	3A7
ATOM	2941	CE2	TRP	408	0.574	-26.677	13.353	1.00	0.00	3A7
ATOM	2942	CE3	TRP	408	-1.619	-26.011	14.121	1.00	0.00	3A7
ATOM	2943		TRP	408		-27.783	14.170	1.00	0.00	3A7
	2944		TRP	408		-27.102	14.983	1.00	0.00	3A7
ATOM.										
MOTA	2945		TRP	408		-27.989	14.995	1.00	0.00	3A7
ATOM	2946	С	TRP	408 -	-3.541	-23.347	10.974	1.00	0.00	3A7
ATOM	2947	0	TRP	408	-3.197	-22.324	10.383	1.00	0.00	3A7
ATOM	2948	N	THR	409	-4.838	-23.556	11.320	1.00	0.00	3A7
ATOM	2949	CA	THR	409		-22.587	11.078	1.00	0.00	3A7
MOTA	2950	CB	THR	409		-23.197	11.275	1.00	0.00	3A7
MOTA	2951	OG1	THR	409		-22.316	10.873	1.00	0.00	3A7
ATOM	2952	CG2	THR	409	-7.503	-23.671	12.727	1.00	0.00	3A7
ATOM	2953	Ċ	THR	409	-5.686	-21.354	11.951	1.00	0.00	3A7
ATOM	2954	0	THR	409		-21.439	13.116	1.00	0.00	3A7
ATOM	2955	N	GLU	410		-20.153	11.363	1.00	0.00	3A7
MOTA	2956	CA	GLU	410		-18.880	11.957	1.00	0.00	3A7
ATOM	2957	CB	GLU	. 410	-6.432	-18.485	13.138	1.00	0.00	3A7
ATOM	2958	CG	GLU	410	-7.920	-18.447	12.751	1.00	0.00	3A7
ATOM	2959	CD	GLU	410	-8.744	-18.043	13.970	1.00	0.00	3A7
ATOM	2960		GLU	410		-18.790	14.985	1.00	0.00	3A7
									0.00	3A7
ATOM	2961		GLU	410		-16.984	13.903	1.00		
ATOM	2962	С	GLU	410	-4.059	-18.872	12.399	1.00	0.00	3A7
ATOM	2963	0	GLU	410	-3.756	-18.654	13.572	1.00	0.00	3A7
ATOM	2964	N	PRO	411	-3.140	-19.188	11.476	1.00	0.00	3A7
ATOM	2965	ÇA	PRO	411		-19.438	11.747	1.00	0.00	3A7
		CD					10.041	1.00	0.00	3A7
ATOM	2966		PRO	411		-19.045				
ATOM	2967	СВ	PRO	411		-19.794	10.370	1.00	0.00	3A7
ATOM	2968	CG	PRO	411	-2.020	-19.039	9.368	1.00	0.00	3A7
ATOM	2969	С	PRO	411	-1.022	-18.216	12.290	1.00	0.00	3A7
ATOM	2970	ŏ	PRO	411		-18.335	12.931	1.00	0.00	3A7
ATOM	2971			412		-17.019	12.058	1.00	0.00	3A7
		N	GLU							
ATOM	2972	CA	GLU	412		-15.791	12.493	1.00	0.00	3A7
ATOM	2973	CB	GLU	412		-14.650	11.516	1.00	0.00	3A7
MOTA	2974	CG	GLU	412	-0.914	-14.895	10.063	1.00	0.00	3A7
ATOM	2975	CD	GLU	412	0.609	-14.849	9.920	1.00	0.00	3A7
ATOM	2976	OE1		412		-15.190	8.807	1.00	0.00	3A7
ATOM	2977	OE2		412		-14.468	10.897	1.00	0.00	3A7
ATOM	2978	С	GLU	412		-15.419	13.903	1.00	0.00	3A7
MOTA	2979	0	GLU	412	-1.079	-14.360	14.405	1.00	0.00	3A7
MOTA	2980	N	LYS	413	-2.226	-16.290	14.589	1.00	0.00	3A7

ATOM	2981	CA	LYS	413	-2.691	-16.035	15.932	1.00	0.00	3A7
ATOM	2982	CB	LYS	413		-16.281	16.093	1.00	0.00	3A7
ATOM	2983	CG	LYS	413		-15.300	15.276	1.00	0.00	3A7
ATOM	2984	CD	LYS	413	-6.569	-15.457	15.519	1.00	0.00	3A7
ATOM	2985	CE	LYS	413	-7.012	-15.075	16.938	1.00	0.00	3A7
MOTA	2986	NZ	LYS	413		-15.230	17.084	1.00	0.00	3A7
ATOM	2987	С	LYS	413		-16.896	16.917	1.00	0.00	3A7
MOTA	2988	0	LYS	413		-18.089	16.718	1.00	0.00	3A7
ATOM	2989	N	PHE	414		-16.288	18.059	1.00	0.00	3A7 3A7
ATOM	2990	CA	PHE	414		-16.968	19.200	1.00	0.00	3A7
ATOM	2991	CB	PHE	414		-15.950 -16.580	20.125 21.179	1.00	0.00	3A7
ATOM	2992 2993	CG	PHE	414 414		-17.214	20.878	1.00	0.00	3A7
ATOM ATOM	2994		PHE	414		-16.541	22.505	1.00	0.00	3A7
ATOM	2995		PHE	414		-17.815	21.887	1.00	0.00	3A7
ATOM	2996		PHE	414		-17.148	23.513	1.00	0.00	3A 7
ATOM	2997	CZ	PHE	414		-17.802	23.199	1.00	0.00	3A7
ATOM	2998	С	PHE	414	-2.045	-17.668	19.981	1.00	0.00	3A7
ATOM	2999	0	PHE	414	-2.819	-17.039	20.697	1.00	0.00	3A7
ATOM	3000	N	LEU	415		-19.006	19.847	1.00	0.00	3A7
ATOM	3001	CA	LEU	415		-19.816	20.488	1.00	0.00	3A7
ATOM	3002	СВ	LEU	415		-20.254	19.504	1.00	0.00	3A7
MOTA	3003	CG	LEU	415		-19.105	18.954	1.00	0.00	3A7
ATOM	3004		LEU	415		-19.603	17.812	1.00	0.00	3A7 3A7
MOTA	3005		LEU	415		-18.424	20.058	1.00	0.00	3A7 3A7
ATOM ATOM	3006	C	LEU	415		-21.064 -22.038	20.998	1.00	0.00	3A7
ATOM	3007 3008	0	LEU PRO	415 416		-21.141	22.271	1.00	0.00	3A7
ATOM	3009	CA	PRO	416		-22.301	22.847	1.00	0.00	3A7
ATOM	3010	CD	PRO	416		-19.967	23.122	1.00	0.00	3A7
ATOM	3011	СВ	PRO	416		-21.888	24.299	1.00	0.00	3A7
ATOM	3012	CG	PRO	416	-0.878	-20.375	24.207	1.00	0.00	3A7
ATOM	3013	С	PRO	416	-2.201	-23.547	22.780	1.00	0.00	3A7
MOTA	3014	0	PRO	416		-24.651	22.766	1.00	0.00	3A7
ATOM	3015	N	GLU	417		-23.381	22.682	1.00	0.00	3A7
ATOM	3016	CA	GLU	417		-24.458	22.678	1.00	0,00	3A7
ATOM	3017	CB	GLU	417		-23.933	22.878	1.00	0.00	3A7
ATOM	3018	CG	GLU	417		-23.126	24.179	1.00	0.00	3A7 3A7
ATOM	3019	CD OF1	GLU	417		-22.672 -23.077	24.323 25.322	1.00	0.00	3A7
ATOM ATOM	3020 3021		GLU	417 417		-21.911		1.00	0.00	3A7
ATOM	3022	C	GLU	417		-25.295	21.427	1.00	0.00	3A7
ATOM	3023	ŏ	GLU	417			21.478	1'.00	0.00	3A7
ATOM	3024	·N	ARG	418		-24.733	20.282	1.00	0.00	3A7
ATOM	3025	CA	ARG	418		-25.279	18.944	1.00	0.00	3A7
ATOM	3026	CB	ARG	418	-3.753	-24.206	17.890	1.00	0.00	3A7
ATOM	3027	CG	ARG	418		-24.508	16.422	1.00	0.00	3A7
ATOM	3028	CD	ARG	418		-24.343	16.069	1.00	0.00	3A7
ATOM	3029	NĘ	ARG	418		-25.466	16.668	1.00	0.00	. 3A7
ATOM	3030	CZ	ARG	418		-25.471	16.670	1.00	0.00	3A7
ATOM	3031		ARG	418		-26.503	17.264	1.00	0.00	3A7
ATOM	3032		ARG	418		-24.456	16.087	1.00	0.00	3A7 3A7
ATOM ATOM	3033 3034	C O	ARG	418 418		-26.538 -26.489	18.706 18.187	1.00	0.00	3A7
ATOM	3035	N	PHE	419		-27.699	19.103	1.00	0.00	3A7
ATOM	3036	CA	PHE	419		-29.076	18.984	1.00	0.00	3A7
ATOM	3037	СВ	PHE	419		-29.565	17.516	1.00	0.00	3A7
ATOM	3038	CG	PHE	419		-29.517	16.915	1.00	0.00	3A7
MOTA	3039	CD1	PHE	419	-5.049	-28.723	15.799	1.00	0.00	3A7
ATOM	3040	CD2	PHE	419		-30.278	17.466	1.00	0.00	3A7
MOTA	3041		PHE	419		-28.691	15.246	1.00	0.00	3A7
MOTA	3042		PHE	419		-30.245	16.919	1.00	0.00	3A7
ATOM	3043	CZ	PHE	419		-29.452	15.806	1.00	0.00	3A7
ATOM	3044	C	PHE	419		-29.334	19.681	1.00	0.00	3A7
MOTA	3045	0	PHE	419		-28.961	19.199	1.00	0.00	3A7 3A7
ATOM ATOM	3046	N	SER	420		-30.000 -30.259	20.861 21.764	1.00	0.00	3A7
ATOM	3047 3048	CA CB	SER SER	420 420		-30.239	23.241	1.00	0.00	3A7
ATOM	3049	OG	SER	420		-30.208	24.172	1.00	0.00	3A7
ATOM	3050	C	SER	420		-31.644	21.508	1.00	0.00	3A7
ATOM	3051	ŏ	SER	420		-32.527	21.013	1.00	0.00	3A7
MOTA	3052	N	LYS	421		-31.842	21.877	1.00	0.00	3A7

ATOM	3053	CA	LYS	421	1.404	-33.112	21.813	1.00	0.00	3A7
ATOM	3054	СВ	LYS	421		-33.196	20.717	1.00	0.00	3A7
								1.00	0.00	3A7
ATOM	3055	CG	LYS	421		-32.380	20.921			3A7
MOTA	3056	CD	LYS	421		-30.845	20.996	1.00	0.00	
ATOM	3057	CE	LYS	421	3.332	-30.147	19.673	1.00	0.00	3A7
MOTA	3058	NZ	LYS	421	1.927	-30.385	19.273	1.00	0.00	3A7
ATOM	3059	С	LYS	421	2.007	-33.350	23.167	1.00	0.00	3A7
ATOM	3060	ō	LYS	421		-32.424	23.962	1.00	0.00	3A7
						-34.620	23.448	1.00	0.00	3A7
MOTA	3061	N	LYS	422						3A7
MOTA	3062	CA	LYS	422		-34.986	24.675	1.00	0.00	
MOTA	3063	СВ	LYS	422		-35.203	25.856	1.00	0.00	3A7
ATOM	3064	CG	LYS	422	2.715	-35.433	27.225	1.00	0.00	3A7
ATOM	3065	CD	LYS	422	3.520	-34.222	27.727	1.00	0.00	3A7
ATOM	3066	CE	LYS	422	4.151	-34.436	29.109	1.00	0.00	3A7
ATOM	3067	NZ	LYS	422		-35.537	29.071	1.00	0.00	3A7
						-36.262	24.379	1.00	0.00	3A7
ATOM	3068	С	LYS	422				1.00		3A7
ATOM	3069	0	LYS	422		-36.483	24.867		0.00	
ATOM	3070	N	ASN	423	3.138	-37.137	23.555	1.00	0.00	3A7
ATOM	3071	CA	ASN	423	3.658	-38.427	23.165	1.00	0.00	3A7
ATOM	3072	CB	ASN	423	2.646	-39.581	23.442	1.00	0.00	3A7
ATOM	3073	CG	ASN	423	1.264	-39.329	22.812	1.00	0.00	3A7
ATOM	3074		ASN	423		-38.476	23.277	1.00	0.00	3A7
							21.734	1.00	0.00	3A7
ATOM	3075		ASN	423		-40.110				3A7
MOTA	3076	С	ASN	423		-38.367	21.703	1.00	0.00	
ATOM	3077	0	ASN	423		-37.323	21.061	1.00	0.00	3A7
MOTA	3078	N	LYS	424	4.481	-39.522	21.148	1.00	0.00	. 3A7
ATOM	3079	CA	LYS	424	4.861	-39.684	19.760	1.00	0.00	3A7
ATOM	3080	СВ	LYS	424	5.998	-40.724	19.591	1.00	0.00	3A7
ATOM	3081	CG	LYS	424		-40.859	18.153	1.00	0.00	3A7
						-41.874	18.013	1.00	0.00	3A7
ATOM	3082	CD	LYS	424						3A7
MOTA	3083	CE	LYS	424		-41.460	18.744	1.00	0.00	
ATOM	3084	NZ	LYS	424		-42.465	18.534	1.00	0.00	3A7
ATOM	3085	С	LYS	424	3.649	-40.125	18.981	1.00	0.00	3A7
MOTA	3086	0	LYS	424	3.011	-41.116	19.335	1.00	0.00	3A7
ATOM	3087	N	ASP	425	3.321	-39.353	17.910	1.00	0.00	3A7
ATOM	3088	CA	ASP	425		-39.492	17.032	1.00	0.00	3A7
ATOM	3089	CB	ASP	425		-40.959	16.658	1.00	0.00	3A7
						-41.005	15.496	1.00	0.00	3A7
ATOM	3090	CG	ASP	425						3A7
ATOM	3091		ASP	425		-41.550	15.698	1.00	0.00	
ATOM	3092		ASP	425		-40.497	14.397	1.00	0.00	3A7
MOTA	3093	Ç	ASP	425	1.009	-38.771	17.679	1.00	0.00	3A7
ATOM	3094	0	ASP	425	0.241	-39.355	18.444	1.00	0.00	3A7
ATOM	3095	N	ASN	426	0.881	-37.457	17.372	1.00	0.00	3A7
ATOM	3096	CA	ASN	426		-36.573	17.945	1.00	0.00	3A7
ATOM	3097	СВ	ASN	426		-35.250	18.487	1.00	0.00	3A7
						-34.458	17.438	1.00	0.00	3A7
ATOM	3098	CG	ASN	426						3A7
ATOM	3099		ASN	426		-34.963	16.848	1.00	0.00	
ATOM	3100	ND2	ASN	426		-33.168	17.234	1.00	0.00	3A7
ATOM	3101	С	ASN	426	-1.189	-36.329	16.915	1.00	0.00	. 3A7
ATOM	3102	0	ASN	426	-1.547	-37.229	16.157	1.00	0.00	3A7
ATOM	3103	N	ILE	427	-1.746	-35.090	16.880	1.00	0.00	3A7
ATOM	3104	CA	ILE	427		-34.709	16.022	1.00	0.00	3A7
ATOM	3105	CB	ILE	427		-33.632	16.647	1.00	0.00	3A7
						-33.389	15.762	1.00	0.00	3A7
ATOM	3106		ILE	427						3A7
ATOM	3107		ILE	427		-34.009	18.097	1.00	0.00	
MOTA	3108	CD .		427		-35.302	18.218	1.00	0.00	3A7
ATOM	3109	С	ILE	427	-2.306	-34.224	14.699	1.00	0.00	3A7
MOTA	3110	0	ILE	427	-2.782	-34.635	13.641	1.00	0.00	3A7
MOTA	3111	N	ASP	428	-1.289	-33.326	14.741	1.00	0.00	3A7
ATOM	3112	CA	ASP	428		-32.752	13.555	1.00	0.00	3A7
ATOM	3113	СВ	ASP	428		-31.262	13.360	1.00	0.00	3A7
						-31.131	13.173	1.00	0.00	3A7
ATOM	3114	CG	ASP	428						
MOTA	3115		ASP	428		-31.683	12.169	1.00	0.00	3A7
MOTA	3116	OD2	ASP	428		-30.473	14.030	1.00	0.00	3A7
ATOM	3117	С	ASP	428	0.815	-32.877	13.650	1.00	0.00	3A7
ATOM	3118	0	ASP	428	1.471	-31.935	14.093	1.00	0.00	3A7
ATOM	3119	N	PRO	429		-34.003	13.251	1.00	0.00	3A7
ATOM	3120	CA	PRO	429		-34.177	13.157	1.00	0.00	3A7
								1.00	0.00	3A7
ATOM	3121	CD	PRO	429		-35.245	12.998			
MOTA	3122	CB	PRO	429		-35.701	13.258	1.00	0.00	3A7
ATOM	3123	CG	PRO	429		-36.266	12.604	1.00	0.00	3A7
ATOM	3124	С	PRO	429	3.490	-33.658	11.858	1.00	0.00	3A7

MOTA	3125	0	PRO	429	2.892	-33.616	10.780	1.00	0.00	3A7
ATOM	3126	N	TYR	430		-33.325	11.967	1.00	0.00	3A7
				430		-33.153	10.884	1.00	0.00	3A7
ATOM	3127	CA	TYR							3A7
ATOM	3128	CB	TYR	430		-34.248	9.770	1.00	0.00	
ATOM	3129	CG	TYR	430		-34.285	8.969	1.00	0.00	3A7
ATOM	3130	CD1	TYR	430	8.048	-34.836	9.516	1.00	0.00	3A7
ATOM	3131	CD2	TYR	430	6.967	-33.566	7.779	1.00	0.00	3A7
ATOM	3132		TYR	430		-34.596	8.926	1.00	0.00	3A7
				430		-33.267	7.232	1.00	0.00	3A7
ATOM	3133		TYR						0.00	3A7
MOTA	3134	CZ	TYR	430		-33.774	7.806	1.00		
ATOM	3135	ОН	TYR	430	10.620	-33.421	7.266	1.00	0.00	3A7
ATOM	3136	С	TYR	430	5.763	-31.761	10.274	1.00	0.00	3A7
ATOM	3137	0	TYR	430	6.683	-31.428	9.529	1.00	0.00	3A7
ATOM	3138	N	ILE	431	4.795	-30.877	10.599	1.00	0.00	3A7
ATOM	3139	CA	ILE	431		-29.502	10.146	1.00	0.00	3A7
							9.784	1.00	0.00	3A7
ATOM	3140	СВ	ILE	431		-28.893				3A7
ATOM	3141		ILE	431		-29.661	8.570	1.00	0.00	
ATOM	3142	CG1	ILE	431	2.477	-28.800	10.949	1.00	0.00	3A7
MOTA	3143	CD -	ILE	431	1.966	-30.124	11.513	1.00	0.00	3A7
ATOM	3144	С	ILE	431	5.480	-28.630	11.193	1.00	0.00	3A7
ATOM	3145	ō	ILE	431		-27.509	10.893	1.00	0.00	3A7
						-29.122	12.460	1.00	0.00	3A7
MOTA	3146	N	TYR	432						
MOTA	3147	CA	TYR	432		-28.443	13.571	1.00	0.00	3A7
MOTA	3148	СВ	TYR	432	5.758	-28.969	14.973	1.00	0.00	3A7
MOTA	3149	CG	TYR	432	4.498	-28.367	15.505	1.00	0.00	3A7
MOTA	3150	CD1	TYR	432	3.438	-29.190	15.886	1.00	0.00	3A7
ATOM	3151		TYR	432		-27.004	15.799	1.00	0.00	3A7
	3152		TYR	432		-28.665	16.575	1.00	0.00	3A7
ATOM									0.00	3A7
ATOM	3153		TYR	432		-26.477	16.484	1.00		
MOTA	3154	CZ	TYR	432		-27.307	16.878	1.00	0.00	3A7
MOTA	3155	OH	TYR	432	1.204	-26.773	17.586	1.00	0.00	3A7
ATOM	3156	C	TYR	432	7.676	-28.741	13.531	1.00	0.00	3A7
MOTA	3157	0	TYR	432	8.161	-29.675	14.169	1.00	0.00	3A7
ATOM	3158	N	THR	433		-27.919	12.778	1.00	0.00	3A7
						-28.119	12.506	1.00	0.00	3A7
MOTA	3159	CA	THR	433						3A7
MOTA	3160	СВ	THR	433		-28.167	10.995	1.00	0.00	
ATOM	3161	OG1	THR	433	9.638	-26.980	10.336	1.00	0.00	3A7
MOTA	3162	CG2	THR	433	9.309	-29.368	10.401	1.00	0.00	3A7
ATOM	3163	С	THR	433	10.729	-27.070	13.107	1.00	0.00	3A7
MOTA	3164	0	THR	433	11.720	-26.744	12.459	1.00	0.00	3A7
ATOM	3165	N	PRO	434		-26.494	14.305	1.00	0.00	3A7
							14.854	1.00	0.00	3A7
ATOM	3166	CA	PRO	434		-25.526				3A7
ATOM	3167	CD	PRO	434		-26.944	15.329	1.00	0.00	
ATOM	3168	CB	PRO	434	10.738	-25.003	16.098	1.00	0.00	3A7
ATOM	3169	CG	PRO	434	9.981	-26.220	16.622	1.00	0.00	3A7
ATOM	3170	С	PRO	434	12.807	-26.180	15.226	1.00	0.00	3A7
ATOM	3171	0	PRO	434	13.809	-25.477	15.300	1.00	0.00	3A7
ATOM	3172	N	PHE	435		-27.518	15.456	1.00	0.00	3A7
						-28.253	15.844	1.00	0.00	3A7
MOTA	3173	CA	PHE	435				•		3A7
MOTA	3174	СВ	PHE	435		-29.173	17.045	1.00	0.00	
ATOM	3175	CG	PHE	435		-28.509	18.358	1.00	0.00	3A7
ATOM	3176	CD1	PHE	435	14.729	-27.557	18.520	1.00	0.00	3A7
MOTA	3177	CD2	PHE	435	12.731	-28.261	19.269	1.00	0.00	3A7
ATOM	3178	CE1	PHE	435	14.264	-26.403	19.460	1.00	0.00	3A7
ATOM	3179		PHE	435		-27.600	20.460	1.00	0.00	3A7
						-26.726	20.695	1.00	0.00	3A7
MOTA	3180	CZ	PHE	435						3A7
ATOM	3181	С	PHE	435		-29.099	14.689	1.00	0.00	
MOTA	3182	0	PHE	435		-29.980	14.855	1.00	0.00	3A7
ATOM	3183	N	GLY	436	13.993	-28.834	13.469	1.00	0.00	· 3A7
ATOM	3184	CA	GLY	436	14.463	-29.495	12.269	1.00	0.00	3A7
ATOM	3185	C	GLY	436		-30.777	12.129	1.00	0.00	3A7
ATOM	3186	ō	GLY	436		-31.061	12.870	1.00	0.00	3A7
						-31.599	11.152	1.00	0.00	3A7
ATOM	3187	N	SER	437						3A7
MOTA	3188	CA	SER	437		-32.872	10.944	1.00	0.00	
ATOM	3189	СВ	SER	437		-32.829	9.974	1.00	0.00	3A7
ATOM	3190	OG	SER	437	11.247	-32.079	10.518	1.00	0.00	3A7
ATOM	3191	С	SER	437	14.585	-33.730	10.351	1.00	0.00	3A7
ATOM	3192	ō	SER	437		-33.291	9.494	1.00	0.00	3A7
ATOM	3193	N	GLY	438		-35.006	10.788	1.00	0.00	3A7
							10.788	1.00	0.00	3A7
MOTA	3194	CA	GLY	438		-36.010				
MOTA	3195	С	GLY	438		-36.414	11.067	1.00	0.00	3A7
MOTA	3196	0	GLY	438	16.526	-36.346	12.293	1.00	0.00	3A7

ATOM	3197	N	PRO	439	17.704 -	36.873	10.443	1.00	0.00	3	A7
ATOM	3198	CA	PRO	439	18.897 -		11.180	1.00	0.00		A7
MOTA	3199	CD	PRO	439	17.653 -		9.152	1.00	0.00		A7
ATOM	3200	CB	PRO	439	19.741 -		10.170	1.00	0.00		A7
MOTA	3201	CG	PRO	439	18.702 -		9.220	1.00	0.00		A7 A7
ATOM	3202	C	PRO PRO	439 439	19.700 - 20.523 -		11.729 12.614	1.00	0.00		A7
ATOM ATOM	3203 3204	О И	ARG	440	19.490 -		11.217	1.00	0.00		A7
ATOM	3205	CA	ARG	440	20.212 -		11.642	1.00	0.00		A7
ATOM	3206	СВ	ARG	440	20.704 -		10.433	1.00	0.00		A7
ATOM	3207	CG	ARG	440	21.775 -		9.617	1.00	0.00	3	A7
ATOM	3208	CD	ARG	440	21.846 -	33.224	8.148	1.00	0.00	3	A7
ATOM	3209	NE	ARG	440	20.618 -	33.741	7.458	1.00	0.00		A7
MOTA	3210	CZ	ARG	440	20.391 -		6.123	1.00	0.00		IA7
ATOM	3211		ARG	440	19.299 -		5.537	1.00	0.00		1A7
ATOM	3212		ARG	440	21.244 -		5.371	1.00	0.00		1A7 1A7
ATOM	3213	C	ARG	440	19.307 - 19.471 -		12.480 12.565	1.00	0.00		BA7
ATOM ATOM	3214 3215	O N	ARG ASN	440 441	18.322 -		13.163	1.00	0.00		BA7
ATOM	3216	CA	ASN	441	17.420 -		14.066	1.00	0.00		8A7
ATOM	3217	СВ	ASN	441	16.263 -		14.515	1.00	0.00		A7
ATOM	3218	CG	ASN	441	16.713 -		15.324	1.00	0.00	3	3A7
ATOM	3219	OD1	ASN	441	17.527 -	35.781	14.869	1.00	0.00	3	3A7
ATOM	3220	ND2	ASN	441	16.154 ~	35.093	16.567	1.00	0.00		3A7
ATOM	3221	С	ASN	441	18.197 -		15.260	1.00	0.00		3A7
ATOM	3222	0	ASN	441	19.263 -		15.550	1.00	0.00		3A7
ATOM	3223	N	CYS	442	17.690 -		15.990	1.00	0.00		3A7
ATOM	3224	CA	CYS	442	18.409 -		17.097 17.676	1.00	0.00		3A7 3A7
ATOM ATOM	3225 3226	CB SG	CYS	442 442	17.629 - 18.592 -		18.905	1.00	0.00		3A7
ATOM	3227	C	CYS	442	18.683 -		18.181	1.00	0.00		A7
ATOM	3228	ŏ	CYS	442	17.779 -		18.699	1.00	0.00		3A7
ATOM	3229	N	ILE	443	19.971 -		18.535	1.00	0.00		3A7
ATOM	3230	CA	ILE	443	20.405 -	32.830	19.531	1.00	0.00	3	3A7
ATOM	3231	СВ	ILE	443	21.872 -	33.211	19.324	1.00	0.00		3A7
ATOM	3232		ILE	443	22.414 ~		20.472	1.00	0.00		3A7
ATOM	3233		ILE	443	22.046 -		17.955	1.00	0.00		3A7
ATOM	3234	CD	ILE	443	21.378 -		17.849	1.00	0.00		3A7 3A7
ATOM	3235	C	ILE	443 443	20.167 - 20.008 -		20.902 21.894	1.00	0.00		3A7
ATOM ATOM	3236 3237	O N	ILE GLY	444	20.106 -		20.975	1.00	0.00		3A7
ATOM	3238	CA	GLY	444	19.894 -		22.204	1.00	0.00		3A7
ATOM	3239	C	GLY	444	18.471 -		22.535	1.00	0.00	3	3A7
ATOM	3240	0	GLY	444	18.222 -		23.479	1.00	0.00	3	3A7 ·
ATOM	3241	N	MET	445	17.493 -		21.788	1.00	0.00		3A7
ATOM	3242	CA	MET	445	16.056 -		21.939	1.00	0.00		3A7
ATOM	3243	СВ	MET	445	15.279 -		21.002	1.00	0.00		3A7
ATOM	3244	CG	MET	445	13.742 -		21.137	1.00	0.00		3A7 3A7
MOTA MOTA	3245 3246	SD CE	MET MET	. 445 445	12.898 - 13.584 -		19.780 20.107	1.00	0.00		3A7
ATOM	3247		MET	445	15.558 -		23.349	1.00	0.00		3A7
ATOM	3248	ŏ	MET	445	14.887 -		23.919	1.00	0.00		3A7
ATOM	3249	N	ARG	446	15.928 -		23.976	1.00	0.00	3	3A7
ATOM	3250	CA	ARG	446	15.476 -	31.910	25.309	1.00	0.00	3	3A7
MOTA	3251	CB	ARG	446	15.826 -		25.684	1.00	0.00		3A7
MOTA	3252	CG	ARG	446	15.490 -		24.538	1.00	0.00		3A7
MOTA	3253	CD	ARG	446	15.588 -		24.911	1.00	0.00		3A7
ATOM	3254	NE	ARG	446	14.428 ~		25.799	1.00	0.00		3A7 3A7
ATOM ATOM	3255 3256	CZ NH1	ARG ARG	446 446	14.005 - 12.921 -		25.986 26.780	1.00	0.00		3A7
ATOM	3257		ARG	446	14.658 -		25.394	1.00	0.00		3A7
MOTA	3258	C	ARG	446	16.001 -		26.348	1.00	0.00		3A7
ATOM	3259	ō	ARG	446	15.276 -		27.248	1.00	0.00		3A7
ATOM	3260	N	PHE	447	17.267 -	30.512	26.201	1.00	0.00		3A7
ATOM	3261	CA	PHE	447	17.865 -		27.113	1.00	0.00		3A7
ATOM	3262	CB	PHE	447	19.408 -		27.061	1.00	0.00		3A7
ATOM	3263	CG	PHE	447	19.952 -		26.613	1.00	0.00		3A7
ATOM	3264		PHE	447	20.810 -		25.520	1.00	0.00		3A7
ATOM	3265		PHE	447 447	19.433 -		27.086 24.778	1.00	0.00		3A7 3A7
ATOM ATOM	3266 3267		PHE	447	20.971 - 19.526 -		26.291	1.00	0.00		3A7
ATOM	3268	CZ	PHE	447	20.229 -		25.096	1.00	0.00		3A7
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MOTA	3269	С	PHE	447	17.285	-28.185	26.918	1.00	0.00	3A7
MOTA	3270	0	PHE	447	17.071	-27.458	27.881	1.00	0.00	3A7
MOTA	3271	N	ALA	448	16.949	-27.798	25.656	1.00	0.00	3A7
MOTA	3272	CA	ALA	448	16.406	-26.493	25.374	1.00	0.00	3A7
ATOM	3273	CB	ALA	448	16.379	-26.216	23.882	1.00	0.00	3A7
MOTA	3274	С	ALA		15.020	-26.344	25.914	1.00	0.00	3A7
ATOM	3275	0	ALA	448	14.679	-25.313	26.493	1.00	0.00	3A7
ATOM	3276	N	LEU	449	14.197	-27.406	25.800	1.00	0.00	3A7
ATOM	3277	CA	LEU	449	12.842	-27.402	26.309	1.00	0.00	3A7
MOTA	3278	CB	LEU	449	12.029	-28.605	25.813	1.00	0.00	3A7
MOTA	3279	CG	LEU	449	11.639	-28.523	24.324	1.00	0.00	3A7
MOTA	3280		LEU		11.120	-29.879	23.807	1.00	0.00	3A7
ATOM	3281		LEU		10.621	-27.401	24.038	1.00	0.00	3A7
MOTA	3282	С	LEU			-27.422	27.811	1.00	0.00	3A7
ATOM	3283	0	LEU			-26.797	28.417	1.00	0.00	3A7
ATOM	3284	N	VAL			-28.111	28.454	1.00	0.00	3A7
ATOM	3285	CA	VAL			-28.171	29.893	1.00	0.00	3A7
ATOM	3286	CB	VAL			-29.213	30.345	1.00	0.00	3A7
ATOM	3287		VAL			-29.141	31.862	1.00	0.00	3A7
ATOM	3288		VAL	450		-30.592	30.049	1.00	0.00	3A7
ATOM	3289	C	VAL	450		-26.828	30.431	1.00	0.00	3A7
ATOM	3290	0	VAL	450		-26.345	31.364	1.00	0.00	3A7
ATOM	3291	N	ASN	451		-26.162	29.833	1.00	0.00	3A7
ATOM	3292	CA	ASN	451		-24.855	30.232	1.00	0.00	3A7
ATOM	3293	CB	ASN	451		-24.401	29.295	1.00	0.00	3A7
ATOM	3294	CG	ASN	451		-25.243	29.476	1.00	0.00	3A7
ATOM	3295		ASN	451		-26.089	30.369	1.00	0.00	3A7
ATOM	3296		ASN	451		-24.981	28.583	1.00	0.00	3A7
ATOM ATOM	3297 3298	0	ASN ASN	451		-23.792	30.150	1.00	0.00	3A7
ATOM	3299	И	MET	451 452		-23.023 -23.759	31.081	1.00	0.00	3A7
ATOM	3300	CA	MET	452		-22.808	29.019	1.00		3A7
ATOM	3301	CB	MET	452		-22.880	28.800 27.353	1.00	0.00	3A7 3A7
ATOM	3302	CG	MET	452		-22.090	26.370	1.00	0.00	3A7
ATOM	3303	SD	MET	452		-22.975	24.894	1.00	0.00	3A7
MOTA	3304	CE	MET	452		-23.810	24.359	1.00	0.00	3A7
ATOM	3305	c	MET	452		-22.982	29.778	1.00	0.00	3A7
ATOM	3306	ō	MET	452		-22.013	30.355	1.00	0.00	3A7
ATOM	3307	N	LYS	453		-24.236	30.042	1.00	0.00	3A7
ATOM	3308	CA	LYS	453		-24.536	30.965	1.00	0.00	3A7
ATOM	3309	СВ	LYS	453	9.864	-26.021	30.868	1.00	0.00	3A7
MOTA	3310	CG	LYS	453	8.486	-26.409	31.399	1.00	0.00	3A7
ATOM	3311	CD	LYS	453	8.218	-27.911	31.258	1.00	0.00	3A7
ATOM	3312	CE	LYS	453	8.280	-28.457	29.817	1.00	0.00	3A7
ATOM	3313	NZ	LYS	453	9.661	-28.675	29.322	1.00	0.00	3A7
ATOM	3314	С	LYS	453	10.616	-24.214	32.386	1.00	0.00	3A7
ATOM	3315	0	LYS	453	9.869	-23.577	33.112	1.00	0.00	3A7
ATOM	3316	N	LEU	454		-24.594	32.812	1.00	0.00	3A7
ATOM	3317	CA	LEU	454		-24.349	34.154	1.00	0.00	. 3A7
ATOM	3318	СВ	LEU	454		-25.110	34.423	1.00	0.00	3A7
ATOM	3319	CG	LEU	454		-26.655	34.462	1.00	0.00	3a7
ATOM	3320		LEU	454		-27.380	34.874	1.00	0.00	3A7
ATOM	3321		LEU	454	•	-27.101	35.377	1.00	0.00	3A7
ATOM	3322	C	LEU	454	_	-22.881	34.440	1.00	0.00	3A7
ATOM	3323	0	LEU	454		-22.383	35.465	1.00	0.00	3A7
ATOM ATOM	3324 3325	N	ALA	455		-22.129	33.501	1.00	0.00	3A7
ATOM	3326	CA	ALA	455		-20.699	33.621	1.00	0.00	3A7
MOTA	3327	CB C	ALA	455 455		-20.149 -19.916	32.468	1.00	0.00	3A7
ATOM	3328	o	ALA ALA	455		-19.316	33.668 34.569	1.00	0.00	3A7
ATOM	3329	N	LEU	456		-20.169	32.730	1.00	0.00	3A7 3A7
ATOM	3330	CA	LEU	456		-19.468	32.642	1.00	0.00	3A7
ATOM	3331	CB	LEU	456		-19.835	31.351	1.00	0.00	3A7 3A7
ATOM	3332	CG	LEU	456		-19.139	30.053	1.00	0.00	3A7
ATOM	3333	CD1		456		-18.619	30.084	1.00	0.00	3A7
ATOM	3334	CD2		456		-20.054	28.836	1.00	0.00	3A7
ATOM	3335	C	LEU	456		-19.770	33.817	1.00	0.00	3A7
ATOM	3336	ŏ	LEU	456		-18.888	34.337	1.00	0.00	3A7
ATOM	3337	N	VAL	457		-21.025	34.323	1.00	0.00	3A7
ATOM	3338	CA	VAL	457		-21.445	35.499	1.00	0.00	3A7
ATOM	3339	СВ	VAL	457		-22.911	35.843	1.00	0.00	3A7
ATOM	3340	CG1		457		-23.325	37.263	1.00	0.00	3A7

ATOM	3341	CG2	VAL	457	7.670	-23.765	34.841	1.00	0.00	3A7
ATOM	3342	C	VAL	457		-20.633	36.694	1.00	0.00	3A7
ATOM	3343	o	VAL	457		-20.161	37.444	1.00	0.00	3A7
ATOM	3344	N	ARG	458		-20.443	36.892	1.00	0.00	3A7
ATOM	3345	CA	ARG	458		-19.722	38.015	1.00	0.00	3A7
	3346	СВ	ARG	458		-19.996	38.164	1.00	0.00	3A7
ATOM	3347		ARG	458		-21.369	38.758	1.00	0.00	3A7
ATOM		CG		458		-21.581	38.977	1.00	0.00	3A7
MOTA	3348	CD	ARG			-21.751	37.641	1.00	0.00	3A7
MOTA	3349	NE	ARG	458				1.00	0.00	3A7
ATOM	3350	CZ	ARG	458		-22.941	37.197		0.00	3A7
MOTA	3351		ARG	458		-22.979	35.995	1.00		3A7
ATOM	3352		ARG	458		-24.080	37.937	1.00	0.00	
ATOM	3353	C	ARG	458		-18.233	37.894	1.00	0.00	3A7
ATOM	3354	0	ARG	458		-17.578	38.869	1.00	0.00	3A7
ATOM	3355	И	VAL	459		-17.640	36.691	1.00	0.00	3A7
MOTA	3356	CA	VAL	459	10.219	-16.217	36.448	1.00	0.00	3A7
MOTA	3357	CB	VAL	459	10.629	-15.894	35.017	1.00	0.00	3A7
ATOM	3358	CG1	VAL	459	10.199	-14.508	34.526	1.00	0.00	3A7
ATOM	3359	CG2	VAL	459	12.165	-16.014	34.950	1.00	0.00	3A7
ATOM	3360	C	VAL	459	8.793	-15.789	36.752	1.00	0.00	3A7
ATOM	3361		VAL	459	8.553	-14.855	37.511	1.00	0.00	3A7
ATOM	3362	N	LEU	460		-16.538	36.226	1.00	0.00	3A7
ATOM	3363	CA	LEU	460		-16.237	36.374	1.00	0.00	3A7
ATOM	3364	CB	LEU	460		-17.011	35.340	1.00	0.00	3A7
				460		-16.588	33.893	1.00	0.00	3A7
MOTA	3365	CG	LEU			-17.596	32.898	1.00	0.00	3A7
ATOM	3366		LEU	460			33.610	1.00	0.00	3A7
ATOM	3367		LEU	460		-15.150			0.00	3A7
ATOM	3368	С	LEU	460		-16.582	37.736	1.00	0.00	3A7
ATOM	3369	0	LEU	460		-16.068	38.141	1.00		3A7
MOTA	3370	N	GLN	461		-17.449	38.498	1.00	0.00	
ATOM	3371	CA	GLN	461		-17.756	39.877	1.00	0.00	3A7
ATOM	3372	CB	GLN	461		-19.025	40.414	1.00	0.00	3A7
ATOM	3373	CG	GLN	461		-19.729	41.554	1.00	0.00	3A7
MOTA	3374	CD	GLN	461		-21.033	41.909	1.00	0.00	3A7
MOTA	3375	OE1	GLN	461		-21.463	41.220	1.00	0.00	3A7
ATOM	3376	NE2	GLN	461	6.464	-21.670	43.029	1.00	0.00	. 3A7
ATOM	3377	С	GLN	461	6.618	-16.632	40.808	1.00	0.00	3A7
ATOM	3378	0	GLN	461	5.945	-16.385	41.809	1.00	0.00	3A7
ATOM	3379	N	ASN	462	7.741	-15.950	40.487	1.00	0.00	3 A 7
ATOM	3380	CA	ASN	462	8.378	-15.014	41.373	1.00	0.00	3A7
ATOM	3381	СВ	ASN	462	9.917	-15.166	41.353	1.00	0.00	3A7
ATOM	3382	CG	ASN	462		-16.436	42.117	1.00	0.00	3A7
ATOM	3383		ASN	462		-17.563	41.666	1.00	0.00	3A7
ATOM	3384		ASN	462		-16.227	43.317	1.00	0.00	3A7
ATOM	3385	C.	ASN	462		-13.582	41.041	1.00	0.00	3A7
ATOM	3386	ŏ	ASN	462		-12.710	41.888	1.00	0.00	3A7
ATOM	3387	N	PHE	463		-13.284	39.807	1.00	0.00	3A7
	3388	CA	PHE	463		-11.906	39.372	1.00	0.00	3A7
ATOM				463		-11.416	38.535	1.00	0.00	3A7
ATOM	3389	CB	PHE	463		-11.494	39.308	1.00	0.00	3A7
ATOM	3390	CG	PHE				38.996	1.00	0.00	3A7
ATOM	3391		PHE	463		-12.474	40.340	1.00	0.00	3A7
ATOM	3392		PHE	463		-10.594 -12.568	39.714	1.00	0.00	3A7
ATOM	3393		PHE	463						3A7
MOTA	3394		PHE	463		-10.684		1.00	0.00	3A7
MOTA	3395	CZ	PHE	463		-11.673	40.747	1.00		3A7
ATOM '	3396	C	PHE	463		-11.715	38.530	1.00	0.00	
MOTA	3397	0	PHE	463		-12.637	37.862	1.00	0.00	3A7
ATOM	3398	N	SER	464		-10.452	38.530	1.00	0.00	3A7
MOTA	3399	CA	SER	464	4.607	-9.95 7	37.639	1.00	0.00	3A7
MOTA	3400	CB	SER	464	3.437	-9.228	38.330	1.00	0.00	3A7
MOTA	3401	OG	SER	464	3.854	-8.156	39.167	1.00	0.00	3A7
ATOM	3402	С	SER	464	5.295		36.654	1.00	0.00	3A7
ATOM	3403	0	SER	464	5.987	-8.102	37.035	1.00		3A7
ATOM	3404	N	PHE	465	5.122	-9.324	35.343	1.00	0.00	3A7
ATOM	3405	CA	PHE	465	5.823		34.275	1.00	0.00	3A7
ATOM	3406	СВ	PHE	465	6.320		33.195	1.00	0.00	3A7
ATOM	3407	CG	PHE	465		-10.312	33.835	1.00	0.00	3A7
ATOM	3408		PHE	465		-11.547	34.451	1.00	0.00	3A7
MOTA	3409		PHE	465	8.689		33.959	1.00	0.00	3A7
MOTA	3410		PHE	465		-12.080	35.204	1.00	0.00	3A7
	3411		PHE	465		-10.176	34.692	1.00	0.00	3A7
ATOM	3411	CZ	PHE	465		-11.399	35.322	1.00	0.00	3A7
MOTA	2416				2.334					

ATOM	3413	С	PHE	465	4.919	-7.687	33.592	1.00	0.00	3A7
ATOM		ō	PHE	465	3.724	-7.936	33.425	1.00	0.00	3A7
ATOM		N	LYS	466	5.493	-6.560	33.115	1.00	0.00	3A7
ATOR	3416	CA	LYS	466	4.734	-5.582	32.382	1.00	0.00	3A7
ATOM		CB	LYS	466	4.290	-4.427	33.296	1.00	0.00	3A7 3A7
ATOM		CG	LYS	466	3.397 2.972	-4.837 -3.643	34.480 35.348	1.00	0.00	3A7
ATOM		CD	LYS LYS	466 466	2.372	-4.046	36.574	1.00	0.00	3A7
ATOM		NZ	LYS	466	2.919	-4.922	37.481	1.00	0.00	3A7
ATON		c	LYS	466	5.602	-5.043	31.290	1.00	0.00	3A7
ATON		0	LYS	466	6.771	-4.756	31.526	1.00	0.00	3A7
ATOM		N	PRO	467	5.061	-4.811	30.080	1.00	0.00	3A7
ATOM		CA	PRO	467	5.708	-4.063	29.024	1.00	0.00	. 3A7 3A7
ATOM		CD CB	PRO PRO	467 467	3.897 4.867	-5.529 -4.318	29.577 27.759.	1.00	0.00	3A7
ATOM		CG	PRO	467	4.104	-5.604	28.064	1.00	0.00	3A7
ATOM		c	PRO	467	5.709	-2.585	29.358	1.00	0.00	3A7
ATOM		O,	PRO	467	4.657	-2.040	29.696	1.00	0.00	3A7
ATOM		N	CYS	468	6.875	-1.912	29.284	1.00	0.00	3A7
ATOM		CA	CYS	468	7.012	-0.524	29.684	1.00	0.00	3A7 3A7
ATOM		CB	CYS	468	8.466 9.057	-0.147 -1.091	30.062 31.487	1.00	0.00	3A7
ATOM ATOM		SG C	CYS	468 468	6.616	0.383	28.544	1.00	0.00	3A7
ATOM		Ö	CYS	468	6.411	1.583	28.713	1.00	0.00	3A7
ATOM		N	LYS	469	6.540	-0.205	27.334	1.00	0.00	· 3A7
ATOM		CA	LYS	469	6.355	0.499	26.104	1.00	0.00	3A7
ATOM		СВ	LYS	469	7.640	0.501	25.281	1.00	0.00	3A7
ATOM		CG	LYS	469	8.757	1.350	25.918	1.00	0.00	3A7 3A7
ATOM		CD	LYS	469 469	10.000 9.788	1.530 2.435	25.028 23.807	1.00	0.00	3A7
ATOM		CE NZ	LYS	469	9.393	3.802	24.218	1.00	0.00	3A7
ATOM		C	LYS	469	5.347	-0.291	25.354	1.00	0.00	3A7
ATOM		0	LYS	469	5.575	-1.459	25.050	1.00	0.00	3A7
ATOM	3446	N	GLU	470	4.138	0.226	25.134	1.00	0.00	3A7
ATOM		CA	GLU	470	3.141	-0.604	24.504	1.00	0.00	3A7 3A7
ATOM		CB	GLU	470	1.701	-0.299 -0.619	24.997 26.491	1.00	0.00	3A7
ATOM		CG CD	GLU	470 470	1.488 1.553	-2.121	26.773	1.00	0.00	3A7
ATOM			GLU	470	1.559	-2.928	25.806	1.00	0.00	3A7
ATOM			GLU	470	1.584	-2.480	27.981	1.00	0.00	3A7
ATOM	3453	С	GLU	470	3.348	-0.317	23.071	1.00	0.00	3A7
ATOM		0	GLU	470	4.315	-0.740	22.429	1.00	0.00	3A7 3A7
ATOM		N	THR	471	2.368	0.501 1.284	22.575 21.360	1.00	0.00	3A7
ATOM		CA CB	THR	471 471	2.447	2.764	21.659	1.00	0.00	3A7
ATOM			THR	471	1.929	3.641	20.661	1.00	0.00	3A7
ATOM			THR	471	3.946	3.049	21.904	1.00	0.00	3A7
ATOM	3460	С	THR	471	2.841	0.808	20.088	1.00	0.00	3A7
ATOM		0	THR	471	3.308	1.608	19.278	1.00	0.00	3A7 3A7
ATOM		И	GLN	472 472	2.875 3.410	-0.535 -1.235	19.884 18.731	1.00	0.00	3A7 3A7
ATOM		CA CB	GLN GLN	472	2.623	-0.915	17.428	1.00	0.00	3A7
ATOM		CG	GLN	472	2.830	-1.913	16.270	1.00	0.00	3 A 7
ATOM		CD	GLN	472	2.412	-3.322	16.703	1.00	0.00	3A7
ATOM	3467	OE1	GLN	472	3.252	-4.222	16.818	1.00	0.00	3A7
ATOM			GLN	472	1.077	-3.502	16.944	1.00	0.00	3A7
ATOM		C	GLN	472	4.893 5.362	-0.974 -0.673	18.547 17.450	1.00	0.00	3A7 3A7
ATOM		O N	GLN ILE	472 473	5.672	-1.090	19.658	1.00	0.00	3A7
ATOM		CA	ILE	473	7.130	-0.993	19.613	1.00	0.00	3A7
ATOM		СВ	ILE	473	7.790	-0.303	20.808	1.00	0.00	3A7
ATOM	3474		ILE	473	9.304	-0.020	20.648	1.00	0.00	3A7
ATOM			ILE	473	7.030	1.009	21.146	1.00	0.00	3A7
ATOM		CD	ILE	473	7.180	2.124 -2.153	20.104	1.00	0.00	3A7 3A7
ATOM		C O	ILE	473 473	7.840 8.886	-2.153	18.619	1.00	0.00	3A7
ATOM		N	PRO	474	7.388	-3.403	19.312	1.00	0.00	3A7
ATOM		CA	PRO	474	8.307	-4.483	19.289	1.00	0.00	3A7
ATOM		CD	PRO	474	6.293	-3.751	20.216	1.00	0.00	3A7
ATOM		СВ	PRO	474	7.554	-5.688	19.660	1.00	0.00	3A7
ATOM		CG	PRO	474	6.580	-5.162	20.707	1.00	0.00	3A7 3A7
ATOM	3484	С	PRO	474	9.042	-4.735	18.043	1.00	0.00	JA /

ATOM	3485	0	PRO	474	8.461	-4.845	16.967	1.00	0.00	3A7
ATOM	3486	N	LEU	475	10.363	-4.780	18.250	1.00	0.00	3A7
ATOM	3487	CA	LEU	475	11.281	-4.868	17.212	1.00	0.00	3A7
ATOM	3488	СB	LEU	475	12.494	-3.929	17.438	1.00	0.00	3A7
MOTA	3489	CG	LEU	475	12.127	-2.431	17.558	1.00	0.00	3A7
MOTA	3490		LEU	475	13.371	-1.592	17.906	1.00	0.00	3A7 3A7
ATOM	3491		LEU	475	11.432	-1.891	16.293	1.00	0.00	3A7
MOTA	3492	C	LEU	475	11.786	-6.229	17.109 18.064	1.00	0.00	3A7
ATOM	3493	0	LEU	475	12.315 11.627	-6.781 -6.792	15.915	1.00	0.00	3A7
ATOM	3494	N CA	LYS LYS	476 476	12.112	-8.088	15.588	1.00	0.00	3A7
MOTA MOTA	3495 3496	CB	LYS	476	11.115	-8.801	14.712	1.00	0.00	3A7
ATOM	3497	CG	LYS	476	9.772	-9.009	15.441	1.00	0.00	3A7
ATOM	3498	CD	LYS	476	8.674	-9.612	14.555	1.00	0.00	3A7
ATOM	3499	CE	LYS	476	8.939	-11.068	14.167	1.00	0.00	3A7
ATOM	3500	NZ	LYS	476	7.894	-11.545	13.235	1.00	0.00	3A7
MOTA	3501	С	LYS	476	13.325	-7.870	14.776	1.00	0.00	3A7
ATOM	3502	0	LYS	476	13.337	-7.042	13.874	1.00	0.00	3A7
MOTA	3503	N	LEU	477	14.395	-8.621	15.042	1.00	0.00	3A7 3A7
ATOM	3504	CA	LEU	477	15.554	-8.551	14.210	1.00 1.00	0.00	3A7
ATOM	3505	CB	LEU	477	16.856 18.083	-8.930 -8.017	14.617	1.00	0.00	3A7
ATOM	3506	CG	LEU LEU	477 477	19.159	-8.239	15.698	1.00	0.00	3A7
ATOM ATOM	3507 3508		LEU	477	18.705	-8.182	13.223	1.00	0.00	3A7
ATOM	3509	C	LEU	477	15.422	-9.412	13.099	1.00	0.00	3A7
ATOM	3510	ò	LEU	477	14.926		13,208	1.00	0.00	3A7
ATOM	3511	N	ARG	478	15.810	-8.885	11.967	1.00	0.00	3A7
ATOM	3512	CA	ARG	478	15.460	-9.604	10.853	1.00	0.00	3A7
MOTA	3513	CB	ARG	478	14.781	-8.647	9.829	1.00	0.00	3A7
MOTA	3514	CG	ARG	478	13.512	-7.955	10.358	1.00	0.00	3A7
MOTA	3515	CD	ARG	478	12.226	-8.561	9.784	1.00	0.00	3A7 3A7
ATOM	3516	NE	ARG	478	12.180		10.198 10.977	1.00 1.00	0.00	3A7
ATOM	3517	CZ	ARG	478	11.186 11.256		11.366	1.00	0.00	3A7
ATOM	3518		ARG	478 478	10.121	-9.764	11.352	1.00	0.00	3A7
ATOM	3519 3520	C	ARG ARG	478	16.502		10.080	1.00	0.00	3A7
ATOM ATOM	3521	ō	ARG .		16.245		8.927	1.00	0.00	3A7
ATOM	3522	N	PHE	479		-10.610	10.632	1.00	0.00	3A7
ATOM	3523	CA	PHE	479		-10.706	9.806	1.00	0.00	3A7
ATOM	3524	СВ	PHE	479	20.076	-10.235	10.539	1.00	0.00	3A7
ATOM	3525	CG	PHE	479	21.147	-9.680	9.633	1.00	0.00	3A7
MOTA	3526		PHE	479	20.917	-8.497	8.929	1.00	0.00	3A7 3A7
MOTA	3527		PHE	479		-10.322	9.495	1.00	0.00	3A7
MOTA	3528		PHE	479	21.894	-7.970 -9.799	8.093 8.652	1.00	0.00	3A7
ATOM	3529		PHE	479 479	23.336	-8.622	7.951	1.00	0.00	3A7
MOTA	3530 3531	CZ C	PHE	479		-12.054	9.251	1.00	0.00	3A7
ATOM ·	3532	0	PHE	479		-12.120	8.413	1.00	0.00	3A7
ATOM	3533	N	GLY	480		-13.153	9.632	1.00	0.00	3A7
ATOM	3534	CA	GLY	480	18.751	-14.416	8.969	1.00	0.00	3A7
ATOM	3535	С	GLY	480		-15.080	9.499	1.00	0.00	3A7
MOTA	3536	0	GLY	480		-14.455	9.781	1.00	0.00	3A7
ATOM	3537	N	GLY	481		-16.400	9.691	1.00	0.00	3A7 3A7
ATOM	3538	CA	GLY	481		-17.199	10.480	1.00	0.00	3A7
MOTA	3539	С	GLY	481		-17.404 -18.530	11.756 12.126	1.00	0.00	3A7
ATOM	3540	0	GLY	481		-16.297	12.120	1.00	0.00	3A7
atom Atom	3541 3542	N CA	LEU	482 482		-16.393	13.801	1.00	0.00	3A7
ATOM	3543	CB	LEU	482		-16.416	14.840	1.00	0.00	3A7
ATOM	3544	CG	LEU	482		-17.132	16.175	1.00	0.00	3A7
ATOM	3545		LEU	482		-16.443	17.020	1.00	0.00	3A7
ATOM	3546		LEU	482		-18.634	15.963	1.00	0.00	3A7
ATOM	3547	С	LEU	482		-15.192	13.998	1.00	0.00	3A7
ATOM	3548	0	LEU	482		-14.069	13.996	1.00	0.00	3A7
ATOM	3549	N	LEU	483		-15.412	14.210	1.00	0.00	3A7 3A7
ATOM	3550	CA	LEU	483		-14.371	14.462 14.069	1.00	0.00	3A7
ATOM	3551	CB	LEU	483		-14.799 -14.905	12.543	1.00	0.00	3A7
ATOM	3552	CG	LEU	483 483		-15.253	12.231	1.00	0.00	3A7
ATOM	3553 3554		LEU	483		-13.634	11.775	1.00	0.00	3A7
MOTA MOTA	3555	CDZ	LEU	483		-14.055	15.923	1.00	0.00	3A7
ATOM	3556	ŏ	LEU	483		-14.926	16.767	1.00	0.00	3A7
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ATOM	3557	N	LEU	484	16.246	-12.778	16.236	1.00	0.00	3A7
					16.374		17.588	1.00	0.00	3A7
ATOM	3558	CA	LEU	484						3A7
ATOM	3559	СВ	LEU	484	17.753	-11.620	17.812	1.00	0.00	
ATOM	3560	CG	LEU	484	18.984	-12.548	17.710	1.00	0.00	3A7
					20.271		17.445	1.00	0.00	3A7
ATOM	3561		LEU	484					0.00	3A7
ATOM	3562	CD2	LEU	484	19.140	-13.413	18.970	1.00		
ATOM	3563	С	LEU	484	15.345	-11.234	17.861	1.00	0.00	3A7
					14.779		16.981	1.00	0.00	3A7
MOTA	3564	0	LEU	484						
MOTA	3565	N	THR	485	15.149	-10.896	19.142	1.00	0.00	3A7
	3566	CA	THR	485 .	14.449	-9.702	19.526	1.00	0.00	3A7
ATOM				•			20.697	1.00	0.00	3A7
ATOM	3567	СВ	THR	485	13.528	-9.902				
ATOM	3568	OG1	THR	485	12.643	-10.981	20.430	1.00	0.00	3A7
ATOM	3569	CG2	THR	485	12.694	-8.634	20.978	1.00	0.00	3A7
						-8.739	19.870	1.00	0.00	3A7
ATOM	3570	С	THR	485	15.542					3A7
ATOM	3571	0	THR	485	16.525	-9.095	20.514	1.00	0.00	
ATOM	3572	N	GLU	486	15.407	-7.491	19.395	1.00	0.00	3 A 7
				486	16.478	-6.537	19.402	1.00	0.00	3A7
ATOM	3573	CA	GLU						0.00	3A7
ATOM	3574	CB	GLU	486	16.229	-5.476	18.329	1.00		
ATOM	3575	CG	GLU	486	16.097	-6.056	16.918	1.00	0.00	3A7
				486	16.045	-4.920	15.900	1.00	0.00	3A7
ATOM	3576	CD	GLU						0.00	3A7
ATOM	3577	OE1	GLU	486	15.044	-4.847	15.140	1.00		
ATOM	3578	OE2	GLU	486	17.014	-4.115	15.863	1.00	0.00	3A 7
			GLU	486	16.763	~5.904	20.729	1.00	0.00	3A7
ATOM	3579	С							0.00	3A7
ATOM	3580	0	GLU	486	17.821	-6.121	21.297	1.00		
ATOM	3581	N	LYS	487	15.871	-5.074	21.275	1.00	0.00	3 A 7
				487	16.181	-4.394	22.523	1.00	0.00	3A7
MOTA	3582	CA	LYS					1.00	0.00	3A7
ATOM	3583	CB	LYS	487	16.681	-2.935	22.345			
ATOM	3584	CG	LYS	487	18.078	-2.831	21.710	1.00	0.00	3A7
		CD	LYS	487	18.582	-1.386	21.553	1.00	0.00	3A7
MOTA	3585							1.00	0.00	3A7
ATOM	3586	CE	LYS	487	17.737	-0.521	20.606			
MOTA	3587	NZ	LYS	487 .	17.683	-1.111	19.249	1.00	0.00	3A7
	3588	С	LYS	487	14.847	-4.380	23.208	1.00	0.00	3A7
MOTA						-3.436	22.965	1.00	0.00	3A7
MOTA	3589	0	LYS	487	14.110					3A7
ATOM	3590	N	PRO	488	14.469	-5.369	24.036	1.00	0.00	
ATOM	3591	CA	PRO	488	13.160	-5.418	24.666	1.00	0.00	3A7
						-6.687	23.995	1.00	0.00	3A7
ATOM	3592	CD.		. 488	15.099					3A7
ATOM	3593	CB	PRO	488	12.772	-6.900	24.541	1.00	0.00	
ATOM	3594	CG	PRO	488	14.103	-7.653	24.646	1.00	0.00	3A7
						-4.931	26.063	1.00	0.00	3A7
MOTA	3595	C	PRO	488	13.285					3A7
ATOM	3596	0	PRO	488	14.207	-5.350	26.760	1.00	0.00	
ATOM	3597	N	ILE	489	12.369	-4.042	26.506	1.00	0.00	3A7
					12.431	-3.564	27.858	1.00	0.00	3A7
ATOM	3598	CA	ILE	489					0.00	3A7
ATOM	3599	CB	ILE	489	12.824	-2.096	28.021	1.00		
ATOM	3600	CG2	ILE	489	14.258	-1.923	27.475	1.00	0.00	3A7
				489	11.831	-1.092	27.392	1.00	0.00	3A7
MOTA	3601	CG1						1.00	0.00	3A7
ATOM	3602	CD	ILE	489	12.182	0.356	27.747			
ATOM	3603	С	ILE	489	11.136	-3.837	28.577	1.00	0.00	- 3A7
	3604	o	ILE	489	10.052	-3.733	28.009	1.00	0.00	3A7
ATOM							29.878	1.00	0.00	3A7
ATOM	3605	И.	VAL	490	11.230	-4.209				3A7
ATOM	3606	CA	VAL	490	10.101	-4.648	30.674	1.00	0.00	
ATOM	3607	СВ	VAL	490	9.925	-6.155	30.572	1.00	0.00	3A7
						-6.911	31.734	1.00	0.00	3A7
MOTA	3608		VAL	490	9.245			1.00	0.00	3A7
ATOM	3609	CG2	VAL	490	9.143	-6.483	29.279			
ATOM	3610	С	VAL	490	10.398	-4.303	32.085	1.00	0.00	3A7
			VAL	490	11.537	-4.064	32.455	1.00	0.00	3A7
MOTA	3611	0						1.00	0.00	3A7
MOTA	3612	N	LEU	491	9.344	-4.289	32.927			
MOTA	3613	CA	LEU	491	9.438	-4.005	34.328	1.00	0.00	3A7
	3614	СВ	LEU	491	8.379	-2.956	34.702	1.00	0.00	3A7
MOTA							35.041	1.00	0.00	3A7
MOTA	3615	CG	LEU	491	8.991					3A7
ATOM	3616	CD1	LEU	491	7.898	-0.495	35.142	1.00	0.00	
ATOM	3617		LEU	491	9.848	-1.615	36.322	1.00	0.00	3A7
				491	9.183		35.064	1.00	0.00	3A7
MOTA	3618	С	LEU						0.00	3A7
ATOM	3619	0	LEU	491	8.303		34.680	1.00		
ATOM	3620	N	LYS	492	9.934	-5.530	36.165	1.00	0.00	3A7
				492	9.855		36.930	1.00	0.00	3A7
ATOM	3621	CA	LYS						0.00	3A7
ATOM	3622	CB	LYS	492	11.254		37.203			
ATOM	3623	CG	LYS	492	12.184	-6.661	38.201	1.00	0.00	3A7
		CD	LYS	492	12.735		37.743		0.00	3A7
ATOM	3624						38.784		0.00	3A7
ATOM	3625	CE	LYS	492	12.568					
MOTA	3626	NZ	LYS	492	11.143	-3.831	38.925			3A7
		C	LYS		9.148		38.247	1.00	0.00	3A7
ATOM	3627									. 3A7
MOTA	3628	0	LYS	492	9.344	-7.295	37.170	1.00	Ų. UU	

ATOM	3629	N	ALA	493	8.315	-5.466	38.338	1.00	0.00	3A7
ATOM	3630	CA	ALA	493	7.783	-4.923	39.576	1.00	0.00	3A7
ATOM	3631	CB	ALA	493	7.164	-3.529	39.347	1.00	0.00	3A7
MOTA	3632	С	ALA	493	6.735	-5.798	40.223	1.00	0.00	3A7 3A7
MOTA	3633	0	ALA	493	5.607	-5.896	39.745	1.00	0.00	3A7
MOTA	3634	N	GLU	494	7.121	-6.449 -7.353	41.348	1.00	0.00	3A7
ATOM	3635	CA	GLU	494 494	6.270 6.221	-8.771	41.447	1.00	0.00	3A7
ATOM ATOM	3636 3637	CB CG	GLU	494	5.073	-9.691	41.921	1.00	0.00	3A7
ATOM	3638	CD	GLU	494		-10.327	43.282	1.00	0.00	3A7
ATOM	3639	OE1		494		-10.984	43.425	1.00	0.00	3A7
MOTA	3640		GLU	494		-10.171	44.193	1.00	0.00	3A7
ATOM	3641	С	GLU	494	6.833	-7.451	43.468	1.00	0.00	3A7
MOTA	3642	0	GLU	494	6.097	-7.692	44.424	1.00	0.00	3A7
MOTA	3643	N	SER	495	8.180	-7.291	43.592	1.00	0.00	3A7 3A7
MOTA	3644	CA	SER	495	9.005	-7.634	44.741	1.00	0.00	3A7
ATOM	3645	СВ	SER	495	10.488	-7.267	44.500 43.315	1.00	0.00	3A7
ATOM	3646	OG	SER	495 495	10.963 8.584	-7.890 -6.990	46.046	1.00	0.00	3A7
ATOM ATOM	3647 3648	С 0	SER SER	495	8.318	-5.791	46.117	1.00	0.00	3A7
ATOM	3649	N	ARG	496	8.506	-7.831	47.102	1.00	0.00	3A7
ATOM	3650	CA	ARG	496	8.050	-7.468	48.419	1.00	0.00	3A7
ATOM	3651	СВ	ARG	496	6.781	-8.270	48.810	1.00	0.00	3A7
ATOM	3652	CG	ARG	496	6.173	-7.918	50.178	1.00	0.00	3A7
ATOM	3653	CD	ARG	496	4.896	-8.715	50.471	1.00	0.00	3A7
ATOM	3654	NE	ARG	496	4.413	-8.345	51.841	1.00	0.00	3A7
MOTA	3655	CZ	ARG	496	3.354	-8.981	52.430	1.00	0.00	3A7 3A7
ATOM	3656	NH1		496	2.955	-8.609	53.681 51.778	1.00	0.00	3A7
ATOM	3657		ARG	496 496	2.696 9.179	-9.982 -7.785	49.356	1.00	0.00	3A7
ATOM ATOM	3658 3659	С 0	ARG ARG	496	9.927	-8.738	49.139	1.00	0.00	3A7
ATOM	3660	N	ASP	497	9.312	-6.984	50.445	1.00	0.00	3A7
ATOM	3661	CA	ASP	497	10.298	-7.171	51.489	1.00	0.00	3A7
MOTA	3662	СВ	ASP	497	10.821	-5.830	52.089	1.00	0.00	.3A7
ATOM	3663	CG ·	ASP	497	9.707	-4.881	52.551	1.00	0.00	3A7
MOTA	3664		λSP	497	8.940	-4.387	51.682	1.00	0.00	3A7
ATOM	3665		ASP	497	9.625	-4.629	53.783	1.00	0.00	3A7 3A7
ATOM	3666	С	ASP	497	9.711	-8.068	52.560	1.00	0.00	3A7
MOTA	3667	0	ASP	497	8.985 10.021	-7.622 -9.384	53.447 52.458	1.00	0.00	3A7
ATOM	3668 3669	N CA	GLU	498 498		-10.423	53.314	1.00	0.00	3A7
MOTA MOTA	3670	CB	GLU	498		-11.610	52.501	1.00	0.00	3A7
ATOM	3671	CG	GLU	498		-11.185	51.557	1.00	0.00	3A7
ATOM	3672	CD	GLU	498	7.253	-12.413	50.822	1.00	0.00	3A7
ATOM	3673	OE1	GLU	498		-12.728	50.989	1.00	0.00	3A7
MOTA	3674	OE2	GLU	498		-13.049	50.081	1.00	0.00	3A7
MOTA	3675	С	GLU	498		-10.918	54.195	1.00	0.00	3A7 3A7
ATOM	3676	0	GLU	498		-10.403	54.157 55.010	1.00	0.00	3A7
ATOM	3677	N	THR	499 499		-11.961 -12.606	55.905	1.00	0.00	3A7
ATOM ATOM	3678 3679	CA CB	THR	499		-12.970	57.245	1.00	0.00	3A7
ATOM	3680		THR	499		-13.726	57.084	1.00	0.00	3A7
ATOM	3681		THR	499		-11.664	57.998	1.00	0.00	3A7
ATOM	3682	С	THR	499		-13.836	55.217	1.00	0.00	3A7
ATOM	3683	0	THR	499		-14.244	54.163	1.00	0.00	3A7
MOTA	3684	N	VAL	500		-14.455	55.826	1.00	0.00	3A7 3A7
MOTA	3685	CA	VAL	500		-15.621	55.300	1.00	0.00	3A7
MOTA	3686	СВ	VAL	500		-15.588 -15.508	55.594 57.109	1.00	0.00	3A7
ATOM	3687		VAL VAL	500 500		-16.768	54.903	1.00	0.00	3A7
ATOM ATOM	3688 3689	C	VAL	500		-16.864	55.847	1.00	0.00	3A7
ATOM	3690	õ	VAL	500		-16.984	57.047	1.00	0.00	3A7
ATOM	3691	N	SER	501	12.542	-17.816	54.939	1.00	0.00	3A7
ATOM	3692	CA	SER	501		-19.059	55.286	1.00	0.00	3A7
MOTA	3693	CB	SER	501		-18.950	55.320	1.00	0.00	3A7
MOTA	3694	OG	SER	501		-20.142	55.806	1.00	0.00	3A7 3A7
ATOM	3695	C	SER	501		-20.035	54.235 54.550	1.00	0.00	3A7
ATOM	3696	0	SER	501 502		-21.094 -19.677	52.947	1.00	0.00	3A7
MOTA	3697 3698	N CA	GLY GLY	502		-20.464	51.805	1.00	0.00	3A7
ATOM ATOM	3699	C	GLY	502		-19.693	51.074	1.00	0.00	3A7
ATOM .	3700	ŏ	GLY	502		-18.585	50.602		0:00	3A7

ATOM	3701	N	ALA	503	14.804	-20.283	50.980	1.00	0.00	3A7
ATOM	3702	CA	ALA	503	15.970	-19.715	50.338	1.00	0.00	3A7
ATOM	3703	СВ	ALA	503	15.775	-19.401	48.838	1.00	0.00	3A7
MOTA	3704	С	ALA	503	16.423	-18.443	51.073	1.00	0.00	3A7
ATOM	3705	OT1	ALA	503	17.016	-18.589	52.175	1.00	0.00	3A7
ATOM	3706	OT2	ALA	503	16.167	-17.323	50.557	1.00	0.00	3A7
TER	3707		ALA	503						
HETATM		FE	HEM	600	19.802	-26.909	18.195	1.00	0.00	HEM
HETATM		NA	HEM	600		-26.973	16.343	1.00	0.00	HEM
HETATM		NB	HEM	600		-25.763	18.746	1.00	0.00	HEM
HETATM		NC	HEM	600		-26.830	20.017	1.00	0.00	HEM
HETATM		ND	HEM	600		-28.034	17.616	1.00	0.00	HEM
HETATM		CIA		600		-27.653	15.248	1.00	0.00	HEM
HETATM		C2A		600		-27.461	14.072	1.00	0.00	HEM
HETATM		C3A		600		-26.605	14.439	1.00	0.00	HEM
HETATM		C4A		600		-26.338	15.849	1.00	0.00	HEM
HETATM		CIB		600		-25.288	17.964	1.00	0.00	HEM
HETATM		C2B		600		-24.465	18.724	1.00	0.00	HEM
HETATM		C3B		600		-24.471	20.029	1.00	0.00	HEM
HETATM		C4B		600		-25.267	20.000	1.00	0.00	HEM
HETATM		CIC		600		-26.220	21.122	1.00	0.00	HEM
HETATM		C2C		600		-26.398	22.303	1.00	0.00	HEM
HETATM		C3C		600		-27.105	21.896	1.00	0.00	HEM
		C4C		600		-27.359	20.473	1.00	0.00	HEM
HETATM		CID		600		-28.419	18.358	1.00	0.00	HEM
HETATM		C2D		600		-29.229	17.581	1.00	0.00	HEM
		C3D		600		-29.362	16.350	1.00	0.00	HEM
HETATM						-28.591	16.366	1.00	0.00	HEM
HETATM		C4D		600 600		-28.392	15.257	1.00	0.00	HEM
HETATM		CHA		600		-25.582	16.615	1.00	0.00	HEM
HETATM		-		600		-25.488	21.097	1.00	0.00	HEM
HETATM		CHC		600		-28.078	19.676	1.00	0.00	HEM
HETATM HETATM				600		-26.027	13.539	1.00	0.00	HEM
		CMA		600		-28.152	12.738	1.00	0.00	HEM
HETATM HETATM		CAA		600		-27.341	11.731	1.00	0.00	HEM
		CBA		600		-28.082	10.424	1.00		HEM
HETATM		CGA O1A		600		-28.897	10.031	1.00	0.00	HEM
HETATM				600		-27.812	9.777	1.00	0.00	HEM
HETATM		O2A CMB		600		-23.749	18.107	1.00	0.00	HEM
HETATM		CAB		600		-23.874	21.208	1.00	0.00	HEM
		CBB		600		-23.138	21.200	1.00	0.00	HEM
HETATM HETATM		CMC		600		-25.906	23.689	1.00	0.00	HEM
				600		-27.556	22.589	1.00	0.00	HEM
HETATM		CAC		600		-27.610	23.914	1.00	0.00	HEM
HETATM		CBC		600		-27.810	18.033	1.00	0.00	HEM
HETATM HETATM		CMD		600		-30.183	15.203	1.00	0.00	HEM
		CBD		600		-30.163	15.127	1.00	0.00	HEM
HETATM						-32.470	14.027	1.00	0.00	HEM
HETATM HETATM		CGD O1D		600 600		-33.625	14.347	1.00	0.00	HEM
				•		-32.020	12.856	1.00	0.00	HEM
HETATM	3/30	02D	LI CALL	600	£3.330	-34.020	12.030	1.00	0.00	******

Sequences:

SEQ ID N°1: P450 Nor, crystal structure 1 rom

SEQ ID N°2: P450 Ery F, crystal structure I oxa

SEQ ID N°3: P450 Terp, crystal structure 1cpt

5 SEQ ID N°4: P450 Cam, crystal structure 3cpp

SEQ ID N°5: P450 BM3, crystal structure 2hpd

The sequence corresponding to the PDB structure includes 471 residues. For more clarity in Figure 1, the last 12 residues have been omitted, the C-terminal part having no equivalent counterpart in the other structures aligned.

10 SEQ ID N°6: P450 2C5, crystal structure 1dt6

Cyp2C5 from Oryctolagus cuniculus (Rabbit), with membrane spanning residues 3-21 deleted and a 4 residue histidine tag at the C-Terminus containing additional internal mutations.

SEO ID N°7: P450 2C5 rabbit

Sequence corresponding to the non-mutated CYP 2C5 gene from Oryctolagus cuniculus (Rabbit), consistently with SwissProt CPC5_RABIT P00179.

SEQ ID N° 8: CYP51, crystal structure 1e9x

Cyp51 from Mycobacterium tuberculosis, with a 4 residue histidine tag at the C-Terminus.

20 SEQ ID N°9: CYP3A1 rat

SEQ ID N°10: CYP3A3 human

Cytochrome P-450, a possible variant of CYP3A4, inducible by glucocorticoids in human liver.

SEQ ID N°11: CYP3A4 human

Numbering starts at Ala 1 (first residue Met is not included, consistently with SwissProt CP34_HUMAN P08684)

SEQ ID N°12: CYP3A5 human

SEQ ID N°13: CYP3A43 human

SEQ ID N°14: CYP3A6 rabbit

SEQ ID N°15: CYP3A7 human

SEQ ID N°16: CYP3A12 dog

SEQ ID N°17: CYP3A29 pig

SEQ ID N°18: CYP3A13 mouse

- Figure 1: Structure-based alignment of human cytochromes P450 3A3, 3A4, 3A5, 3A7 and 3A43 and of selected mammalian P450 3A isozymes, with bacterial P450 crystal template structures and rabbit P450 2C5 crystal template structure.
- Sequence numbering is indicated for each enzyme of the structural template and for the human 3A4 and 3A7 isozymes, as examples given in the present invention. This alignment is first based on the structural alignment of bacterial P450s and rabbit P450 2C5 derived from GOK analysis. Human P450 3A sequences were then aligned with in-house tools that locates the CSBs on the target sequence. The alignment shown outside the CSBs is not relevant, as there is no structural information available in these regions. The CSB sequences are indicated by bold uppercase characters and are highlighted in grey. Amino acids strictly conserved between CYP3A and 2C5, or between CYP3A and all the sequences of crystal structures, are highlighted in black.
- 15 Figure 2: Ramachandran plot of a lowest energy model of CYP3A4 produced by DYANA-XPLOR calculations from the six-template structural alignement. Figure 3: view of one optimized CYP3A4 model. This figure can be replaced by the whole set of coordinates file of table 3 in the PDB format.
- Figure 4: final position of testosterone into the CYP3A4 and CYP3A7 active sites after soft-restrained dynamics docking. The active sites are characterized by six Substrates Recognition Sites (SRS, after Gotoh 1989, in bold) associated to fragments of secondary element structures (in italic).
 - Panel 4A In CYP3A4 active site, the docked testosterone molecule is oriented so that the A steroid cycle (carrying in position 3 a carbonyl function with an oxygen atom symbolized by a large ball) is close to the heminic iron. This supports the propensity of CYP3A4 to metabolize testosterone in 6 β position as indicated by the black solid arrow.
 - Panel 4B In CYP3A7 active site, the docked testosterone molecule is oriented so that the D steroid cycle (carrying in position 17 a hydroxylic function with an oxygen atom symbolized by a large ball) is close to the heminic iron. This supports the propensity of CYP3A7 to metabolize testosterone in 16 α position as indicated by the black solid arrow

Figure 5: Energy profile of the soft-restrained dynamics docking of testosterone into CYP3A4 model.

Example 1: Determination of the 3D-structure of P450 3A4.

Material

The coordinates of the six P450 crystal structures: P450cam (3cpp), P450terp (1cpt), P450BM-3 (2hpd), P450eryF (1oxa), P450 nor (1rom) and P450 2C5 (1dt6) were retrieved from the Brookhaven Protein data bank. The structural alignment and the conserved regions determination were realized using the GOK software (Jean et al. 1997) running on an Octane Silicon-Graphics workstation. Structures were built using the DYANA (Güntert et al. 1997), and X-PLOR softwares (Brünger 1992). Docking studies were performed with SYBYL 6.6 (Tripos Inc.) and TRIPOS force field. The structures were analyzed using Procheck-NMR (Laskowski et al. 1993) and visualized under SYBYL 6.6 (Tripos Inc.).

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Common Structural Blocks (CSB) determination.

The first key point of this homology modeling study is the identification of the structural elements (hereafter designed as CSBs for Common Structural Blocks) conserved among the family of cytochromes P450 of known 3D structures, and the localization of these elements in the target sequence. These two tasks are performed using the GOK software (Jean et al. 1997), and are well described in a forthcoming article (Minoletti et al., Proteins, Structure, Function and Genetics, 2002). In brief, the basic idea of CSB identification by GOK is to use an internal coordinate representation – (α, τ) in our case (another representation of ϕ , ψ and ω angles) – and to search for fragments in the six-template proteins having similar local trajectories in the internal coordinate space. GOK provides two adjustable parameters (the α -mesh and the α -margin) that define the tolerance on the comparison of the trajectories. These parameters were adjusted recursively to values ranging from 15 to 30° (α-mesh) and 1 to 3 (α-margin in mesh units). The evaluation of the quality of the match was measured using two multiple-way rmsd calculated in the cartesian coordinates space: mp-rms (the mean of all pairwise rms deviations) and s-rms (the mean of the deviations calculated with respect to a mean structure obtained from the average internal coordinates). For the different CSBs, mp-rms value ranged between 0.3 and 4.9 Å in average, and s-rms between 0.04 and 2.4 Å.

CYP3A4 sequence alignment and evaluation of the profile

The multiple sequence alignment derived from the CSB identification was then used to build a similarity profile. The profile is defined as a position-specific scoring table created from aligned gap-free segments such as CSBs (Jean et al. 1997). The alignment then consists in a search of the best match (as per the best score) between a CSB of sequences defined structurally (i.e. independently of the nature of the aligned residues) and several other sequences that are well-aligned and exhibit a high sequence identity. In the P450 3A subfamily, many proteins exhibit high sequence identity. We extended our profile search program to take this information into account, i.e. to align the profile with a pre-defined multiple alignment of the cytochromes P450 3A subfamily members sequences (Gotoh 1992; Nelson et al. 1996). The similarity score was calculated using BLOSUM62 matrix (Henikoff and Henikoff 1992). The in-house tool SmartConsAlign (Atelier de Bioinformatique, Université Paris VI) described in Jean et al. 1997, allows to move the consensus matrix along the multiple sequence alignment of P450 3A family, and computes for each position a score of similarity. The best alignment found of CYP3A4 on CSBs is shown in Figure 1.

Once the alignment is completed, the 3D model rebuilding process can incorporate the atom Cartesian coordinates of the template structures only for amino acids located in structurally conserved regions (i.e. the CSBs). The coordinates of any of the template structures can be used for determining the final template. In each CSB, amino acid positions have been renumbered according to the sequence of human P450 3A4. At a given position, when residues are identical between all the template structures and the target sequence, the 3D coordinates of the reference residues are purely assigned to the modeled (target) residue. When residues differ, only the coordinates of the backbone atoms are assigned (Cα), and sometimes Cβ when they exist. Side chains are rebuilt from libraries giving the most probable rotamers for each amino acid (see below). In some cases, it was possible to superimpose the positions of carbon atoms of lateral chains up to ranks γ and δ along the sidechain, thus explicitly defining a unique rotamer.

For amino acids located outside the CSBs (structurally variable zones that include generally loops), the rebuilding is more complex, and can be done only after rebuilding of structurally conserved zones. In the multiple structural alignment (Figure 1), the regions separating the CSBs bring no structural information at all. Short loops are rebuilt entirely, since solutions of acceptable geometry for atoms are in limited number, *i.e.* the lowest energy drives the selection of the good geometry. For longer segments, various structures are provided by the constrained minimization runs, and a manual selection is operated.

10 Constraints derivation and rebuilding

A strategy inspired of the techniques commonly used to built structures from NMR data (Patard et al. 1996) is applied. The main idea is to express all available information issued from the comparison of the templates in term of geometrical constraints (distances and angles). Each constraint will be defined as an interval (for a given pair of atoms, this is the average of the six atom-atom distances found in the template structures +/- the standard deviation), similarly to the strategy developed by Havel and Snow (Havel and Snow 1991). However, the number of constraints corresponding to all atom-atom distances, for example, would be prohibitive for a protein of the size of the P450 (around 1,000,000 inter-residual distances if we consider 250 conserved residues and an average of four atoms per residues). Previous NMR studies (Patard et al. 1996) have shown that local constraints are sufficient to allow a correct reconstruction of a structure. This reduces drastically the number of constraints needed, and increases the flexibility of the model. In addition, similarly to what is done in protein structure determination by NMR, we can build a family of structures instead of a single model. This allows an easier analysis of the well or less well-predicted regions. This is also an advantage for the analysis of the side-chain positions, particularly in prevision of a substrate docking study. Finally, the loops are passively reconstructed with the rest of the structure. The only specific information we have introduced in variable regions was to guide all their residues to an allowed region of the Ramachandran diagram. Indeed, analysis of well-defined structures shows that nearly all residues, including those of the loops, should belong to an allowed region. The lower the proportion of residues

found outside the allowed Ramachandran regions, the better the structure is. This criterion of quality has been applied to derive the model described herein.

Accordingly, we retained for model rebuilding all the distance and angle intervals corresponding to the following principles:

- all distances for which the lower boundary was less than 8 Å. This cutoff is totally sufficient to ensure, at least, the formation of the local structure elements. Such a cutoff is relatively high and thus costly in terms of size of constraints file, but proved necessary to ensure good results for the P450s. This may be due to the fact that P450 enzymes are mostly formed of α-helices, the average distance between two helices being larger than between two adjacent β-strands. In addition, the percentage of residues located outside CSBs is rather high in the structural alignment of P450s, and a better convergence can be obtained only at the expense of a high number of rebuilding distance constraints.
 - all the distances involving at least one side-chain atom, to preserve the spatial arrangement between CSBs
 - finally, all the distances involving atoms of the heme group, to fix as much as possible the neighborhood of the iron atom.

The total number of distance constraints was, in these conditions, equal to 58506. Similarly, angular constraints were calculated in each building block. A CSB is indeed defined as a conserved trajectory in the φ, ψ coordinates space (or α, τ). Thus, dihedral angles φ and ψ of all residues located in CSBs can be defined as constraints, given by the average values of corresponding φ, ψ angles in the six templates +/- the standard deviation. To these backbone dihedral angles, can be added the side chains torsion angles χ_1, χ_2 whenever possible, as determined by the rotamer selection. The total number of dihedral angle constraints was, in these conditions, equal to 761.

Rotamer selection

In proteins, the preferential orientation of the side chain (60°, -60°, 180°) depends on the local conformation of the residue, and thus on the nature of the secondary structure in which the residue is involved. According to the rotamer library built by Karplus and coll. (Dunbrack and Karplus 1993), to a given (φ, ψ) couple in the

Ramachandran diagram can be associated a specific rotamer for each type of residue. These tables have been used to determine the most probable rotamer for each residue located in CSB, except when there are conserved atoms in the side chain that assign unambiguously a rotamer (χ_1, χ_2) . The selected (χ_1, χ_2) couples were included in the above-mentioned set of angle 761 dihedral constraints.

Structure calculation and optimization

We used a procedure similar to structure calculation starting from NMR constraints. A first set of structures was calculated using the DYANA software (Güntert et al. 1997) and the 58506 distance and 761 angular constraints. Families of structures are generated. The energy of each structure is minimized with the procedure vtfmin in DYANA.

Due to the size and the amount of loops in the molecule, some structures presented topological defects and were discarded. The others were further optimized by using the X-PLOR software. A set of constraints was added at this stage in order to guide the loop residues to the nearest allowed region in the Ramachandran diagram. The topology and parameter files of CHARMM22 were used. The electrostatic term was turned off.

The DYANA software is unable to deal with disconnected objects. A new residue type was, thus, added to the standard amino acid library to take into account the the presence of the heme. This residue was obtained by combining the heme to a cysteine and was inserted at position 441 in the sequence of the protein (Figure 1).

Description of the CYP3A4 Model

We rebuilt a model of the protein depleted of its first 50 residues (N-terminal domain). This segment is highly hydrophobic, and supposed to form the anchor of the protein in the membrane. There is no structural information about this putative transmembrane domain, and this segment was thus not incorporated into the modeling process, and in the final model. Such a "free" segment (with no constraints) would perturbate the convergence of computation or the stability of the whole rebuilt structure.

The quality of the various structures optimized under XPLOR was checked for the stereochemical quality (backbone and side chain conformation) by PROCHECK

(Laskowski et al. 1993). The Ramachadran plot shows that our six-template approach generated converging models, possessing the same fold. The lowest energy models had 73% of their non-glycine and non-proline residues with φ , ψ conformation in the most favoured regions of the Ramachandran plot (core region), 20% in additional allowed regions, and 5% in the generously allowed regions. Only 2.3% (9 residues) had their φ , ψ conformation in disallowed regions (Figure 2). The total number of residues in the model is 452; which 399 are non-glycine and non-proline residues, and number of residues in the native sequence is 502.

When compared to the CYP2C5 crystal structure, it can be noticed that the CYP3A4 model exhibits a good 3D similarity in the global fold than expected, since this structure counts only for one in the six-template approach. This proves that in this approach, there is no "averaging" effect, *i.e.* the mammalian structure had a decisive influence over the five bacterial (and fungus) templates. Our final fold of CYP3A4 is very consistent with a mammalian one, despite the fact that it has been rebuilt by using the structural information contained in non-mammalian cytochromes P450.

The active site is delimited by the six substrate recognition sites (SRS) that have been first identified and described by Gotoh (Gotoh 1992) from the unique structure available in the early 1990s (P450cam), and that are today commonly accepted for depicting substrate recognition by various cytochromes P450 (especially from the family 2, but extended to other P450 families). These sites are associated with the active site and are located in the less conserved regions of the CYPs, thus possibly accounting for the various substrate specificity among P450s. When comparing our various optimized structures, it is found that SRS1 (100-125, includes helix B), SRS 2 (205-218, includes C-terminus of helix F), and SRS3 (237-249, includes Nterminus part of helix G) are located in less-defined regions, with significant variability in spatial position (flexibility). These regions correspond also to parts of the sequence that are less well-aligned. At the opposite, the SRS4 (295-320, central part of helix I), SRS5 (363-380, C-term of helix K and β-sheet β1-4) and SRS6 (470-490, β -sheets β 4-1 and β 4-2) are well-defined fragments of the structures. SRS4 and SRS5 segments in particular are correlated to regions in the sequence that are unequivocally aligned.

The only model structure of CYP3A4 that has been described in the literature and that we can handle for structural comparison, is that of Szklarz and Halpert, derived from a multiple-template approach (four-bacterial template) (Szklarz and Halpert 1997). Roughly, the same secondary structures are identified, but we found divergences in SRS location between their model and those derived from the present approach. SRS4 and SRS5 match well, but SRS2 is shifted (divergence in the position of helix F along the sequence), while SRS1 (helix B'), SRS3 (helix G) and SRS6 (sheet β4) are more notably displaced. The loops connecting the secondary structures of these SRS significantly disagree. These differences are likely to issue from a wrong alignment with the crystal P450 structures in the model of Szklarz and Halpert.

Example 2: Determination of the 3D-structure of P450 3A7.

The model rebuilding of CYP3A7 was performed according to the techniques described above in example 1 for CYP3A4, except that we used a restrained set of four-template structures, still including the mammalian CYP2C5, in order to test the robustness of the modeling approach. Below are pointed out only the differences in input data and the results relevant to CYP3A7.

20 Material

The coordinates of the four P450 crystal structures: P450BM-3 (2hpd), P450eryF (10xa), P450 51-like from *Mycobacterium tuberculosis* (1e9x) and P450 2C5 (1dt6) were retrieved from the Brookhaven Protein data bank and used as initial template for GOK analysis.

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Common Structural Blocks (CSB) determination.

The GOK parameters were adjusted recursively to values ranging from 10 to 30° (α -mesh) and 1 to 3 (α -margin in mesh units). Occasionally, the α -mesh value was pushed up to 60° to refine some local structured loops (DE loop, HI loop) or short helices (such as J'). 27 CSBs have been identified. New CSBs were detected: the block 7* (between blocks 6 and 7A), the block 7B* (between 7B and 8) and the block 7C (between 7B* and 8). For the different CSBs, mp-rms value ranged between 0.12 and 4.57 Å in average.

The best alignment found of CYP3A7 on CSBs is shown in Figure 1. On the 459 residues comprised in the model structure (the protein was rebuilt depleted of its first 44 residues from the N-terminal domain), 337 residues were found located in CSBs, i.e. 73% of residues belong to structurally conserved regions of the four-template set.

Constraints derivation and rebuilding

With a larger cutoff (12 Å), we obtained around 73000 distance constraints, and 900 dihedral constraints.

The residue covalently linked to the heme group is at position 442 in the sequence of the protein (Figure 1).

Description of the CYP3A7 model

The four-template approach generated converging models, possessing the same fold. The PROCHECK analysis for structure quality assessment for the lowest energy models showed 74.4% of their non-glycine and non-proline residues with φ , ψ conformation in the most favoured regions of the Ramachandran plot (core region), 18.2% in additional allowed regions, and 4.7% in the generously allowed regions. 2.7% (11 residues) had their φ , ψ conformation in disallowed regions. The total number of residues in the model is 459; which 407 are non-glycine and non-proline residues, and number of residues in the native sequence is 503.

A closer inspection of the structure, and after the results of dynamics docking experiments (see below), revealed that several hydrogen bonds can hinder the main access to the active site. Thus, key residues that are likely to be involved in the recognition and admission of the substrate are Q79; F102; R105; R106; F108; F248; F304 and E374, and additionally C98 and C377 (Figure 4B). More specifically, R105, R106, Q79 and E374 can establish mutual hydrogen bonds in one of the access channels, and are thus involved in the access of the substrate towards the active site.

Example 3: Docking Strategy

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Our aim in this example was to obtain the different positions of the known substrates of CYP3A in the active site, consistent with the oxidation sites and

biochemical differences among the CYP3A isoforms. Considering the fact that the heme-binding site is deeply buried in the protein structure, and thus the selection and the pathway of the substrates within the enzyme structure are strongly dependent on the various possibilities of structure opening, we implemented a special approach more appropriate to flexible structures, hereafter referred as "restrained dynamics docking" or "soft-restrained dynamics docking". This technique employs constrained molecular dynamics simulations, where the only constraints are heme-substrate distances. The successive steps are:

10 Conversion of the PDB XPLOR file in PDB for SYBYL file

The optimized structures with XPLOR (PDB format) are visualized with the SYBYL 6.6 software (Tripos Inc.), which implies a conversion of the file (atoms types correction) so as to make it compatible and exploitable in the constrained dynamics which will be performed with SYBYL.

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Stabilization of the P450 3A4 model generated under XPLOR

Then, we do agregate N°1 (in the meaning of SYBYL) with all the $NC_{\alpha}CO$ atoms of the peptide backbone of the protein. The structure is relaxed with a dynamic of 10ns at 100K followed by a minimization of 100 steps. Agregate N°1 is then deleted.

We do agregate N°2 constituted of the protein C_{α} only. The protein relaxation is reiterated with a dynamic of 10 ns at 100K and a minimization of 100 steps. Agregate N°2 is then deleted.

The all protein is then relaxed with a first dynamic of 1ns at 100K, followed by a dynamic of 1ns at 200K and a dynamic of 10ns at 300K. We terminate with a minimization of 100 steps.

Restrained dynamics docking of the substrate (example: testosterone)

We do agregate N°3 constituted of all atoms outside a sphere of 20Å around the C_{α} of residues constituting the heart of the B' loop. We also add heminic iron to this aggregate.

The substrate is placed inside the protein, at around 30Å from the heminic iron and next to SRS1 and SRS5 sites. The substrate is placed so that the contraints between

the heminic iron and the substrate backbone go between SRS1, SRS5 and SRS3. Thus, for testosterone docking, we establish 4 distance contraints (limit below 3Å, above 10Å) between heminic iron and C3, C8, C10 and C13 carbons with a constraint of 2 kcal/Å on the entire structure so as to avoid to favour the approach of one part of the substrate more than the other.

We begin to perform a dynamic without contraints of the entire system at 20 K during 2ns to stabilize the system, then we perform a dynamic under contraints at 20 K during 5ns. We observe that the substrate worms between SRS1, SRS3 et SRS5 to reach a position at the vicinity of heminic iron. We terminate with a dynamic without contraints at 300 K to relax the system and we realize a minimization of 1000 steps.

Results

We found that the testosterone molecule is positioned at the vicinity of heminic iron in such way that the C6 of testosterone be at 4.9Å of the iron, which is compatible with the hydroxylation of this compound to give 6β -hydroxy-testosterone (Figure 4A).

Minimizations and dynamics with the SYBYL software are performed with the Tripos force field following the parameters: dielectric constant equal to 1 and distance-dependent, minimization method of POWELL, a minimum gradient of 0.05kcal.mol⁻¹.Å⁻¹, electrostatics charges calculated according to the Gasteiger-Hückel method, and a NB cutoff of 8.0Å (non-bond energies). The energetic diagram of dynamic docking of testosterone is shown in Figure 5.

25 Interest of this docking strategy:

Most P450 isozymes recognize only one substrate (for specific catalysis in a metabolic pathway), or a very limited number of substrates, all chemically closely related. At the contrary, CYP 3A isozymes are known to recognize a large palette of substrates, and are also capable of multiple binding in the active site, up to three molecules in the vicinity of the heme, according to the model developed by Hosea et al. 2000. Multiple pharmacophoric behavior (Ekins et al. 2003), as well as allosteric or synergistic effects, characterize the members of this P450 subfamily.

The docking strategy described above can be easily extended to different binding and metabolism scenario.

For example, the docking of two or three testosterone molecules, or of two testosterone molecules and one alpha-naphtoflavone molecule (αNF) can be simulated in the following manner:

- In a first step, a testosterone molecule is dynamically docked under constraints, and then released of its constraints to freely evolve in the active site and find a first bound equilibrium position.
- In a next step, an external testosterone is presented, at the same entrance of the protein structure or in the vicinity of another access channel, and then dynamically docked under constraints. The system first evolves under constraints applied to the second molecule, and can be released for a subsequent free MD simulation of the two molecules bound in the active site. One can see the first bound molecule (testosterone or another substrate) to be re-oriented under the effect of the second docking, simulating a situation of cooperativity.
- Similarly, the second molecule docked can be different from the first bound, e.g. a first testosterone bound to the active site followed by the docking of an αNF molecule, or the reverse situation.
- One can combine of course the possibilities: for example, two molecules (identical or of different chemical nature) are docked following the two steps above, and then, after stabilization around an equilibrium position, a third molecule is introduced under constraints, and then released from its constraints to let the system evolving towards a favorable energetic conformational state. In this way, two αNF and one testosterone or one αNF and two testosterone can be docked.
- Of course, not only substrates can be docked, but also inhibitors. The docking procedure above can help to measure the potential inhibitory power of a molecule, for example a compound comprising an imidazole group. A first step would include a standard constrained dynamic docking of the potential inhibitor, followed by a free MD simulation (constraints are released when the inhibitor is in the active site), or by a specifically-constrained MD simulation where the imidazole group is confined in the vicinity of the heminic iron by using an additional distance constraint Fe-imidazole. In a following step, a second substrate is dynamically docked under constraints from the exterior, and one can determine in what

conditions the second molecule can chase the first one from its binding position. The strength of the additional constraint can be a measurement of the inhibitory potential.

Correspondingly, the exit pathway of the metabolites can be explored by simulating the exit of the molecule bound to the active site, using either free MD simulation (if the chemical nature of the transformed molecule allows an energetical instability), or using inverted constraints, *i.e.* soft distance constraints (between an external point and the bound molecule) that help to expel out the metabolite. Additionally, the best exit pathway can be deduced from the most favored energy profiles.

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Claims

- 5 1. A method for designing a 3-dimentional (3-D) model of a protein, the 3-D representation of at least three family members has already been experimentally obtained, [said 3-D representation presenting similarities], comprising the steps of:
 - a. identification of common structural blocks (CSBs) among said members of said family,
- b. alignment of the amino-acids primary sequence of said family members according to said structural similarities, represented by said CSBs, in order to obtain a first alignment,
 - c. alignment of said protein as compared on said first alignment, in order to obtain a second alignment, wherein:
- i. alignment of said protein is performed in order to optimize the amino-acids alignment between said protein and said first alignment, when one or more consensus amino-acid exists in said aligned CSBs in said first alignment, and in the amino-acid sequence of said protein, said consensus amino-acids are anchors of said second alignment,
- 20 ii. no insertion or deletion of amino-acids can be performed in the aligned CSBs, wherein insertion or deletions are possible in out-of-block regions, if better to align the primary amino-acids sequences,
 - d. definition of the 3-D structure of CSBs of said protein, according to the 3-D structure of the CSBs of said family members,
- e. definition of the global constraints (distance and angular constraints) derived from the comparisons of the structural templates in CSBs, and definition of the local constraints (distance and angular constraints) for the atoms of residues that are not structurally determined after step d. (that are not in the CSBs),
 - f. selection of rotamers,
- 30 g. determination of a family of 3-D model structures of said protein, taking into account said 3-D structure of CSBs obtained in step d., said global and local constraints defined in step e., and said rotamers defined in step f.,
 - h. optimization of said family of 3-D models obtained in step g., by

- i discarding structures that present topological defects, and
- ii recalculating 3-D structures by taking electrostatic forces into account, and performing the method again from step c. downward, with modifications in the alignment between the primary sequence of said protein and said first alignment,
- when the obtained model structures do not satisfactorily account for known mutations having biological effects.
 - 2. The method of claim 1, wherein said 3-D representation of family members has been obtained by crystallography or NMR.
- 3. The method of claim 1, wherein said alignment of said CSBs in step b. is performed by use of the GOK software.
 - 4. The method of claim 1, wherein said alignment of said CSBs in step c. is performed by use of the GOK software.
 - 5. The method of claim 1, wherein step d. is performed according to the following rules:
- 15 i. at a given position, when residues are identical between all the template structures and the target sequence, the 3D coordinates of the reference residues are purely assigned to the target residue,
 - ii. When residues differ, only the coordinates of the backbone atoms are assigned $(C\alpha)$, and sometimes $C\beta$ or $C\gamma$ when they exist.
- 20 6. The method of claim 1, wherein said definition of local constraints in step e. is performed by analysis of the allowed regions in Ramachandran diagram.
 - 7. The method of claim 1, wherein global and local constraints are selected in step e. by the following rules:
 - i. all distances for which the lower boundary was less than 8 Å.
- 25 ii. all the distances involving at least one side-chain atom, to preserve the spatial arrangement between CSBs
 - iii.all the distances involving atoms of any active group such as an heme group, to fix as much as possible the neighborhood of said active group, such as an iron atom.
- 30 8. The method of claim 1, wherein angular constraints are selected in step e. by the following rule:

- i. dihedral angles φ and ψ of all residues located in CSBs are defined as constraints, given by the average values of corresponding φ, ψ angles in said family members +/- the calculated standard deviation.
- 9. The method of claim 1, wherein said rotamers in step f are selected from the couples according to the tables of Dunbrack and Karplus, where the choice of rotamers of a given amino acid is guided by the most favored zones in Ramachandran χ_1 , χ_2 maps.
- 10. The method of claim 1, wherein said step g. is performed with the DYANA software.
- 10 11. The method of claim 1, wherein said optimization in step h. comprises the use of the X-Plor software, as described in A. T. Brunger, X-PLOR, version 3.1.
 - 12. The method of claim 1, wherein said protein is a cytochrome P450 subfamily 3A comprising mammal and human cytochromes P450 3A.
- 13. The method of claim 12, wherein said mammal cytochrome P450 3A is
 5 selected from the group comprising CYP3A6 (SEQ ID N°14), CYP3A12 (SEQ ID N°16), CYP3A29 (SEQ ID N°17) and CYP3A13 (SEQ ID N°18).
 - 14. The method of claim 12, wherein said human cytochrome P450 subfamily 3A is selected from the group comprising CYP3A4 (SEQ ID N°11), CYP3A7 (SEQ ID N°15), CYP3A5 (SEQ ID N°12) and CYP3A43 (SEQ ID N°13).
- 15. The method of claims 1 and 14, wherein said family members that are used for performing said first alignment for designing a 3-D model of CYP3A4 are chosen from Nor (SEQ ID N° 1), Ery F (SEQ ID N° 2), terp (SEQ ID N° 3), Cam (SEQ ID N° 4), BM3 (SEQ ID N° 5) and 2C5 (SEQ ID N° 6).
- 16. The method of claims 1 and 14, wherein said family members that are used for performing said first alignment for designing a 3-D model of CYP3A7 are chosen from Ery F (SEQ ID N° 2), BM3 (SEQ ID N° 5), CYP51 (SEQ ID N° 8) and 2C5 (SEQ ID N° 6).
 - 17. A 3-D structure model of a protein, obtained by the method according to claim 1.
- 30 18. The model of claim 17, wherein said protein is a cytochrome P450 subfamily 3A comprising mammal and human cytochromes P450 3A.

- 19. The model of claim 18, wherein said mammal cytochrome P450 3A is selected from the group comprising CYP3A6 (SEQ ID N°14), CYP3A12 (SEQ ID N°16), CYP3A29 (SEQ ID N°17) and CYP3A13 (SEQ ID N°18).
- 20. The model of claim 18, wherein said human cytochrome P450 subfamily 3A is selected from the group comprising CYP3A4 (SEQ ID N°11), CYP3A7 (SEQ ID N°15), CYP3A5 (SEQ ID N°12) and CYP3A43 (SEQ ID N°13).
 - 21. The model of claim 20, wherein said protein is a cytochrome P450 3A4 or 3A7.
- The model of claim 21, wherein the residues C97; R104; F101; F107; F247;
 F303 and C376 are involved in the CYP 3A4 for the recognition and uptake of the substrate at the entry site, and its binding into the active site.
 - 23. The model of claim 20, wherein the residues Q79; F102; R105; R106; F108; F248; F304 and E374 are involved in the CYP 3A7 for the recognition and uptake of the substrate at the entry site, and its binding into the active site.
- 15 24. The model of claim 22, having the 3-D atomic coordinates of Table 3.
 - The model of claim 23, having the 3-D atomic coordinates of Table 4.
 - 26. A method for designing a protein, biological functions of which are altered, comprising:
 - a) obtaining a 3-D model of said protein by the method of claim 1,
- b) analyzing said model of step a., and determining the amino-acids that are putatively involved in the biological functions of said protein,
 - c) changing said amino-acids by mutating the corresponding nucleotides on the nucleic acid sequence coding for said protein, in order to obtain a mutated protein having altered properties.
- 25 27. A computer-assisted method for performing restrained dynamics docking of a substrate on an enzyme, a 3-D structure of which is available, comprising the steps of
 - j. determining a force field, and independently simulating the presence of said enzyme in said force field,
- 30 k. minimizing the potential energy (Ep) linked to said force field of said 3-D structure, wherein the spatial position of some atoms of said enzyme is fixed, and wherein the other atoms are mobile, by allowing mobility of the mobile atoms, by i. simulating an increase in temperature (in order to give kinetic energy),

- ii. and minimizing the potential energy by re-specifying the temperature as 0 Kelvin (K)
- 1. optionally repeating step k in order to obtain other Ep minima, wherein said Ep minima are such that the structure of the protein remains folded,
- 5 m. minimizing Ep in said force field of said 3-D structure, wherein all the atoms of the protein are mobile, by
 - i. simulating an increase in temperature (in order to give kinetic energy), and
 - ii. minimizing the potential energy by re-specifying the temperature as 0 Kelvin (K)
 - n. simulating, at 0 K the presence of said substrate next to said enzyme,
- o. optionally generating a molecular dynamics simulation on said substrate and enzyme (simulating an increase in temperature, in order to allow mobility of the atoms)
 - p. generating some constraints to said substrate, in order to impose that it has interaction with said enzyme,
- q. generating a molecular dynamics simulation on said substrate and enzyme, with said constraints imposed in step p.,
 - r. optionally, generating a molecular dynamics simulation on said substrate and enzyme without said constraints of step p.
- 28. The method of claim 27, wherein said fixed atoms in step **k**, are the backbone atoms N-Cα-CO in the first minimization step and only Cα in subsequent minimization steps.
 - 29. The method of claim 27, wherein said kinetic energy is simulated by temperature increase to about 100 K for about 5-20 ns.
 - 30. The method of claim 27, wherein said force field in step j. comprises forces linked to
 - a. the distance between atoms,
 - b. the angles of valence,
 - c. the dihedral angles,
 - d. the deformation with regard to planar geometry,
- 30 e. the electrostatic field,
 - f. the Van der Waals forces,
 - g. hydrogen bonds.

- 31. The method of claim 27, wherein said constraints in step **p**. are attraction constraints to force said substrate in the active site, and wherein said constraints are not prejudiced to the exact spatial conformation of the substrate in the active site.
- 32. The method of claim 31, wherein said constraints are final distance constraints between some atoms of said substrate and some atoms of amino-acids present in said active site.
 - 33. The method of claim 27, wherein step o. is performed with a simulated temperature of between about 15 and 50 K.
- 34. The method of claim 27, wherein step q. is performed with a simulated temperature of between about 15 and 50 K.
 - 35. The method of claim 27, wherein step r. is performed with a simulated temperature of between about 200 and 350 K.
 - 36. The method of claim 27, wherein said enzyme is a cytochrome P450 subfamily 3A comprising mammal and human cytochromes.
- 15 37. The method of claim 36, wherein said cytochrome is a cytochrome P450 3A4, and said structure is the structure obtained by the method of claim 15, in particular the model structure of claim 22.
 - 38. The method of claim 36, wherein said substrate is a small organic compound which size can range for example from MW 288 (testosterone) to MW 1203 (cyclosporine A).
 - 39. The method of claim 38, wherein said substrate is testosterone.
 - 40. A computer-assisted method for performing restrained dynamics docking of at least two substrates on an enzyme, a 3-D structure of which is available, comprising the steps consisting of performing the steps depicted in claim 27 with a first substrate and repeating said steps with a second substrate when the first substrate reaches an unconstrained state after molecular dynamics simulation..
 - 41. The method of claim 40, wherein the first and second substrates are the same molecule.
 - 42. The method of claim 40, wherein the first and second substrates are different molecules.
 - 43. The method of claim 41, wherein the first and second substrates display an allosteric effect.

- 44. The method of claim 41, wherein the first and second substrates display a synergistic effect.
- 45. The method of claims 41 and 42, wherein at least one of the substrates is an inhibitor or display an inhibitor-based mechanism.
- 5 46. The method of claims 41 and 42, wherein at least one of the substrates is an agonist.
 - 47. The method of claim 40 comprising successively repeating the steps of claim 20 with a 3rd, 4th or 5th substrate, some of them being the same or different molecules.
- 10 48. The method of claim 40, wherein said fixed atoms in step k. are the backbone atoms N-Cα-CO in the first minimization step and only Cα in subsequent minimization steps.
 - 49. The method of claim 40, wherein said kinetic energy is simulated by temperature increase to about 100 K for about 5-20 ns.
- 15 50. The method of claim 40, wherein said force field in step **j**. comprises forces linked to:
 - a. the distance between atoms,
 - b. the angles of valence
 - c. the dihedral angles,
- 20 d. the deformation with regard to planar geometry,
 - e. the electrostatic field,
 - f. the Van der Waals forces
 - g. hydrogen bonds
 - 51. The method of claim 40, wherein said constraints in step **p.** are attraction constraints to force said substrate in the active site, and wherein said constraints are not prejudiced to the exact spatial conformation of the substrate in the active site.
 - 52. The method of claim 51, wherein said constraints are final distance constraints between some atoms of said substrate and some atoms of amino-acids present in said active site.
- 30 53. The method of claim 40, wherein step o. is performed with a simulated temperature of between about 15 and 50 K.
 - 54. The method of claim 40, wherein step q. is performed with a simulated temperature of between about 15 and 50 K.

- 55. The method of claim 40, wherein step r. is performed with a simulated temperature of between about 200 and 350 K.
- The method of claim 40, wherein said enzyme is a cytochrome P450 subfamily 3A comprising mammal and human cytochromes P450 3A.
- 5 57. The method of claim 56, wherein said cytochrome is cytochrome P450 3A4, and said structure is the structure obtained by the method of claim 15, in particular the model structure of claim 22.
 - 58. The method of claim 40, wherein said first and second substrates are small organic compounds which size can range from MW 288 (testosterone) to MW 1203 (cyclosporine A).
 - 59. The method of claim 58, wherein said substrate is testosterone.
 - 60. The use of the method according to claim 27 or 40 for screening, designing or identifying natural, unnatural substrates or substrate analogs, as well as inhibitors, activators or modulators of said enzyme.
- 15 61. The use of the method according to claim 40 or 47 for determining the effect of a first substrate on a second substrate.
 - 62. The use according to claim 61 applied to pharmaceutical products.
 - 63. The use of the method according to claim 40 or 47 for determining the effect of a first testosterone molecule on a second testosterone molecule.
- 20 64. The use of the method according to claim 40 or 47 for determining the effect of a first testosterone molecule on a second alpha-naphtoflavone molecule.
 - 65. The use of the method according to claim 27 to 47 for determining the oxidative modification of the substrate according to the proximity to the heme of a part of the substrate.
- 25 66. The use of the method according to claim 27 to 39, or 40 to 47, for performing dynamic docking of the said metabolite, either in the absence or in the presence of the second substrate in the computed simulation.
 - 67. The use of the method according to claims 27 to 39, or 40 to 47, to compare the energy of the bound metabolite relatively to the energy of its parent substrate bound, in order to determine if the exit of the given metabolite from the enzyme is favored or not.

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4 Cam (3cp)	1)	ecid ongurabibb	ikempqpktf gelknlpll	. ;	21	
5 BM3 (2hpc 6 2C5 (1dt	5)	makkt	sskgklpen teffiigni		25	
7 CPC5 RABIT	mdpv vvlvlg	lcci lllsiwkans	grgkl-page tafaiigni		43	
8 cyp51 (1e9:					22	
9 CP31 RAT	dllsaltlet wvllav					•
10 CP33 HUMAN	alipdlamet wlllav					
11 CP34 HUMAN	alipdlamet wlllav				50)
12 CP35 HUMAN	mdlipnlavet wlllav					
13 C343 HUMAN	mdlipnfamet wvlvat	slvl lyiygthshk	lfkklging teleflgti			
14 CP36 RABIT	mdlifslet wvllaa	slvl lylygtsthg	lfkkmqipom tolifiqti			
15 CP37 HUMAN	mdlipnlavet wlllav	slil lylygtrthg	lfkklgigge teleflgna ifrklgigge telefvgta	(51)
16 CP3C_CANFA	mdlipsfstet wlllai:	slvl lylygtythg	ifrklgipgs telefvgta			
17 CP3T_PIG	mdlipgfstet wvllat	slvl lylygtyshg	lfkklgigg rellyfgni	i		
18 CP3D_MOUSE	mdlipnfsmet wmllat	slvl lylygthshg	ifkklgimm kalaflgti	1		
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1	eppAEFA-KLRAt-	n PVSQVKLE ag	SLAWLVIKHK DVCFVatse	- (58	-
2	dWYST YAZUre	ta PVTPVRFE-g	qDAWLYTGYD EAKAAlsdl	- (54	
3	d-evIYPA-FKWLrd	ed Brawanikda	dPMWIATKHA DVMQIgkqp	, (68	
4	gVOEA WAVI qe	sund Dramittend-	-GHWIATRGO LIREA yedy		79 67	
5	t-d-k-PVOA-LMK Lad	el-d Kirkrey-d	rVTRYLSSOR LIKEAC-des	• (73	•
6	qidakdisks=LTKFse	grg- PVETVILGIIK	- TVVLHGYE AVKEA vdl		91	
7	qidakdisks LTRFse	gag - PVFTVILGIIK	kovvilsgshanefff-ra	7 /	66	
8	r-t-d-giguemokyrd	ec-d pretrong-d	-ELFAITDTE MIKNV Vec	• `	00	′
9 10	nyy-mgrake byechk	kad- KAMCEADGOU	-EVLAITOPD MIKLV vke	- -		
11	syn-kgrCMR DMRChk	kog KVWGEYDGag	-EVLAITDPD MIKTV	= (97)
12	Syn-KgECME: DIECUK	WG KMWGTYEGO	- VIAITOPD VIRTVIVE	• `	•	•
13	ful-ralWNF DREChe	kwa- EMWGLYEGaa	-PMLVIMDPD MIKTV vke	2		
14	evr-kgTWDF DIECrk	kwa- KMWGLFDGra	-ELMVITOPD MIKTVIIVke	3		
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16 17	gyr-ngFYVF DMKCfs gyr-kgVDHF DKKCfq	ogg- KMWGVYDGrq	- ELLAVIDPN MIKSV置vke	3		
16	gyr-ng FYVF DMKC fs gyr-kg VDHF DKKC fq ayq-kg FWEC DIQC hk	dga- kwmeraderd dga- kwmeraderd	-EVLAITOPD IIKTVIIvke	3		
16 17	gyr-ngFYVF DMKCfs gyr-kgVDHF DKKCfq	ogg- KMWGVYDGrq	- ELLAVIDPN MIKSV置vke	3		
16 17	gyr-ng FYVF DMKC fs gyr-kg VDHF DKKC fq ayq-kg FWEC DIQC hk	dga- kwmeraderd dga- kwmeraderd	-EVLAITOPD IIKTVIIvke	3		
16 17	gyr-ngffvf DMKCfs gyr-kgvDHF DKKCfq ayq-kgfwEC DIQChk CSB 1*	afig- kmwgvydgrq kmg- kmwglydgrq CSB 1**	-EVLAITOPN MIRSVEVACE -EVLAITOPD IIRTVEVACE CSB 1			
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16 17 18	gyr-ngffVF DMKCfs gyr-kgVDHF DKKCfq ayq-kgFWEC DIQChk CSB 1* klskvrtrqg rlssdpkkky pgveve	fpel SASGKOA fpay lgfgEDVRN-	CSB 1		94)
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16 17 18 1 2 3 4 5 6 7	gyr-ngfYVF DMKCfs gyr-kgVDHF DKKCfq ayq-kgFWEC DIQChk CSB 1* klskvrtrqg rlssdpkkky pgveve lfsnae hfssecp rfdknleefagr eefagr ddldq	fpel SASGKQA fpay lgfpedvrn- gse ilyddineag SALKFV SALKFV SALKFV SALKFV SALKFV SALKFV SASGKQA SASGKQA	aka -kpTFYDMD CSB 1 ay fatMGTSD mrsisggch vidSLTSMD		94 10 10 91 98 11) 7) 5)))
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1 2 3 4 5 6 7 8 9 10 11	PEHMHORS MVEPTETPEA VKnLOPYLLORTVDDLLEG MKOKGCANGP PTHTRIRK LVSQEETVIT VEAMR PRVEQITAEL LDEVGdS-GV PTHTAYRG LTINWEGPAS ir KLEEN GRILOASVOR ILDF-dge PEOROFA: LANGUVGMPV Vd KLENG GRILOASVOR ILDF-dge PEOROFA: LANGUVGMPV Vd KLENG GRILOASVOR ILDF-dge PEOROFA: LANGUVGMPV Vd KLENG GRILOSSIES: LRPQgq PEOROFA: LANGUVGMPV Vd KLENG GRILOSSIES: LRPQgq PEOROFA: LANGUVGMPV VG ASP PEOROFA: LANGUVGMPV LRPG ASP PEOROFA: LANGUVGMPV LRPG	(150) (147) (138) (145)
13 14 15 16 17 18	EDERRYT LLSPTFtsg- klEMLPII AQYGDVNVKN LRQEaekgkpEMLRISTELSETEtsg- klEMUPITEAQYGDVLVRN-LRREaetgkpEMLRIT LLSPTFttg- klEMFPII GQYGDVNVN LRKEaekgkaEMLRIT LLSPTFtsg- klEMFPII SHYGDLUVSN LRKEaekgkpEMLRIT LLSPTFtsg- rlEMFPII NQFTDVLVRN MRQGlgegkp CSB 2A CSB 2B	(169)
1 2	VDLVKEFALP VPSYMIYTLL GVPFNDLEVI TOONATRI ng VDIVDRFAHP LETKY CELL GVDEAARCAN GRVSSELL vm	(177) (176)
3	COPMUDCATY YPLHWWITAL GVE EDDEPLY LKLTODEEGV	(190)
Δ	CNETEDYAEP-EPIREMELA GLP EEDIPHL KYLTDOMTIP	(187)
5	TEVPEDMTRITTLDTEGLCGT NYRfnsfyrd qphPFITSMV RALDEAMNkl cDPTFILGCA PCNVCSVIS HNRfdykdEEFLKLM ESLHENVEll	(188)
	CDPTFILGCA PCNYICSVIE HNRfdykdEEFLKIM ESLHENVEll	(190)
7	COPTFILGCA PCNVICSVIE HNRfdykdEEFLKLM ESLNENVRI1	(208)
8	IDELDFFARE TIYTSSACLIEGIKFrd qldgrfakty HelergTDpl	(179)
9	VTMKKVFGAY SMDVATSTSE GVNVdslnNPKDPFV EKTKKLLRfd VTLKDVFGAY SMDVATSSSE GVNVdslnNPQDPLV ENTKKLLRfd	
10	VILKOVEGAY SMOVETSTS GVNidsl-n NPODPFV ENTKKLLRfd	(213)
11	VTIKDIFGAY SMDVHTGTSE GVNidsl-n NPQDPFV ESTKKFIKfg	(213)
12	TITED FEAT MANUFACTE CIVIL del NEODEFI KNMKKLLK d	
13 14	INLKDFFGAY TMDVTTGTLE GVNldslnNPQDPFL KNMKKLLKld VDLKEIFGAY SMDVTTGTSE GVNidslrNPQDPFV KNVRRLLKfs	
15	VILKHVEGAY SMD VETSTSE GVSidsln NPODPEV ENTKKLLRfn	(214)
16	INLKDVFGAY SMDVUTSTSE GVNidslnHPQDPFV ENTKKLLKfd	,
17	VIMKDIFGAY SMDVATSTAE GVNidslnNPQDPFV ENSKKLLKfs	
18	TSMKDIFGAY SMDYTATSE GVNidslnNPQDPFV EKIKKLLKfd	
	CSB 3 - CSB 4	
1	s stareASAAN=OELLDYLAIL VEORLY	(204)
2	dp eraegrooas REVVNFIIDL VERRRT	(204)
3	eaarrFHETIEATFYDYFNGF:TVDRRS	(216)
4	dg smtFAEAK EALYDYLIPI IEORRO	(213)
5	qranpdd -payd enkrqFOEDI KYMNDLVDKI IADRKAs	(226)
6	gtpwlqvynn fpalldyfp- gihktLLKNA-DYIKNFIMEK VKEHOK1-ld	(238)
7	sspwlgyvnn fpalldyfp- gihktLKNA DYIKNFIMEK VKEHEK1-ld	(256)
8	avvdpvl -pi esfrrnear NGIVALVADI MNGRIAnp	(216)
9	ffdplfls vvlfpfltpi yemlnICMFP KDSIEFFKKF VYRMKEtrld	
10	fldpffls itvfpflipi levlnICVFP REVTNFLRKA VKRMKEsrle	
11	fldpffls itvfpflipi levlnICVFF REVINFLRKS VKRMKEsrle	(261)
12	fldplfls iilfpfltpv fealnVSLFP KDTINFLSKS VNRMKKsrln	
13	fld-pflll islfpfltpv fealnIGLFP KDVTHFLKNS IERMKEsrlk	
14	ffd-pllls itlfpfltpi fealhISMFP KDVMDFLKTS VEKIKDdrlk	
15	pldpfvls ikvfpfltpi lealnITVFP RKVISFLTKS VKQIKEgrlk	(262)
16	fldpfffs illfpfltpv feilnIWLFP KKVTDFFRKS VERMKEsrlk	
17	ffdpflls liffpfltpi fevlnITLFP KSSVNFFTKS VKRMKEsrlt	
18	ifd-plfls vtlfpfltpv fdalnVSLFP RDVISFFTTS VERMKEnrmk	
	CSB 5	

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6 TRST-MAYSI HAWK-HEEV AARVOED er vigrhrs-pc mqdrsrmpyr (327	
7 TESTIMANSE LIMIK-HEEV AARVOE EMET VIGINIS-PC moders in the control of the contr	345	•
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9 PTSSTTSFVL HSTAT-HTDT OKKLOREIGH alpnka-ppt ydtylomewil		
10 TESVESTIM YERAT-HEDV QQKLOEFSIGA VIDAKA-PDT YGTVIQMERI 11 TESSVESTIM YERAT-HEDV QQKLOEFSIGA VIDAKA-PDT YGTVIQMERI	355)
12 TESVESTIL YETAT-HEDV QQKICKE da vlpnka-ppt ydavvqmExiL		
13 TESTTEPFIM YELAT-HEDV QQKLQE da vlpnka-pvt ydalvqmEmL		
14 TISSTESFIM HLEAT-HEDV QQKLGE dt llpnke-lat ydtlvkmEVL		
15 THE SVESTIL TELEVICORVER dt vlpnka-ppt ydtvlql	356)
16 TESTSESFIM YEGAT-FEDV QOKLGE Eda tfpnka-lpt ydalvqmemi		
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2 DDTUDEAURW TAPUK - FMR TARADTEURG - ONIKRGDRI-MUSIPSANKD (332	
	328	-
5 GMYLNEALRI WPTAD-afSI TAREDTVLGG eTPLEKGDEL MVLIFOLHRU	363 376	
O CONTRACTOR OF THE PROPERTY O	394	-
7 EAVIHEIQRE IDLLptnlph AVTRDVRERN -YFIERGIDI ITSLTSVLHD (8 ENVLRETLEL HPPLi-ilms Vakgefevog -HRIHEGDLV AASPAISNRI (355	
9 DMVLNETLEL YPIGnr-ler VCKKDVEING -VFMPKGSVV MIPSYALHRD		
10 BMVVNETLRL FPIAMI-LER VCKKDVEING -MFIRKGWVV MIPSYALHRD		
11 DMVVNETLRL FPIAMT-1ER VCKKDVEING -MFIEKGWVV MIPSYALHRD (403)
12 DMVVNETLRL FPVAir-ler TCKKDVEING -VFIPKGSMV VIPTYALHHD		
13 DMVVNETLRL FPVVSI-VTR VCKKDIEING -VFIPKGLAV MVPIYALHHD		
14 DMVVNETLRL YPIAGT-1ER VCKKDVDING -TFIEKGTIV MMPTYALHRD 15 DMVVNETLRL FPVAMT-1ER VCKKDVZING -MFIEKGVVV MIPSYVLHHD (404)
The same of the sa	1	•
17 DMVVNETLRL YPIAAr-ler ACKKDVEIHG -VFV <u>PKG</u> TVV VVPVFVLHRD		
18 PMVVNETLEL YPIAGI-1ER VCKTDVEING -LFIEKGTVV MIPTFALHKD		
CSB 8 CSB 9 CSB 10		

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1	EEVE-RNEDE ENMork	wppq-delegegegdhrc laehlakael	(3	62	.)	
2	PSON-POPHR EDVITCH	trgHELSEGOGIHFC MGRPLAKLEG	(3	60)	
3		- TENUTARING TENUTARIEM	(3	371	.)	
4	POPM_ACOMH VDESTG	k-v-sharteghgshie Lgohlarrei	(3	167)	
5	WITH THE RESERVE	k-v-shillegigshic icohilarei aipqh-abikpegigorac icoprilie -gnfkksdymmbaackwc vcechawei -gnfkksdymmbaackwc vcechawei qedlinrwtwiipegaakwc vcaarimoi	(4	110)	
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14	POHW-TEPDE ERBETISKEN	Kuninpy-11 Herenders Town Print	1 1	152		
15	PKYW-TEDEK ELHERISKKN	Kanlaby-11-12-GSU2-CC TANKE	, ,			
1.6	OSLW-PEREE BREETISTKN	Kdsinpy-ti LPEGIGPKNG IGHKEHIMUM				
17	PDLW-PEREE ERBeriskkh	kdtinpy-ty LPEGTOPENC ISMRFALMIM				
18	PKYW-PEEEE EREerfskkn	dazubh-mr negograng rengentar				
	CSB 10 CSB 11	CSB 12A CSB 12B				
•	mmrremt VAVE BDDT KVav	plgwnyrpianrdygryddp <u>ay</u> if		(403)
1	PURIDAT POPULATION	ad-DVVWRRS LilRGIDHLP Vrldg			403	-
2	EXTERNAL DE L'EVELOGE	PPRLVAT NEVGGPKNVP-Irftka		i	412)
3	ATTENDED TO A TO	gA010HKSEGIvSGVOALF Lvwdpattka	v	•	414	-
4	TVITALWITA-LOOPSIDE	-n-yelDIREHTLtLRPEGEV.Vkakskkipl	ggip			
5	TLYCOMMENT	pkdIDITAVV NGTVSVPPSY Olcfipi	hhhh	ì	473	Ś
6	FLETTSTEON - ALOSIVE	pkdlDITAVV NGTVSVPPSY Olcfipi	***********	ì	487	'n
7	LIMISITED W-KIOSIVE	p-eSYRNDHS KMVVQLAQPACCVryrritgv			450	
8	KAIFSVILKE: I - EFENDOD	tq-IPLKLSR QGILQPTKPI Ilkvvpr		•		•
9	KLANTKVION H-SPOPCKE	tq-IPLKLSL GGllQPEKPV Vlkvesr				
10	KLANIKVION WSFRECKE	tq-IPLKLSL-GGllOPEKPV-Vlkvesrdgt	vsga	1	502	١
11	KLANIKVLON III SIKPEKE	tq-IPLKLDT QGliQPEKPI Vlkvdsrdgt	lege	`		•
12	KTATIKATANE SEKECKE	tq-IPLKLDN LPLLQPEKPI Vlkvhlrdgi	tsan			
13			cogp			•
	KLAVIRALONEE—SFKPCke	te mister och operat Vikuserdai	iraa			
14	KLALVRIMON SE SFKLCke	tg-VPLKLGK OGILQPEKPI Vlkvvsrdgi	irga	,	503	١
15	KLALVRIMON F SFKLCke	tq-VPLKLGK QG1LQPEKPI Vlkvvsrdgi tq-IPLKLRF GG1LLTEKPI Vlkaesrdet	irga vsga	(503)
15 16	KLALVRIMON F SFKLCKE KLALVRVI ON F SFKPCKE KLALVRVI ON F SFKPCKE	tq-VPLKLGK QGllQPEKPI Vlkvvsrdgi tq- <u>IPLKLRF GGllLTEKPI V</u> lkaesrdet tq-IPLKLNA QGlIQPEKPI Vlkveprdgs	irga vsga vnga	(503)
15 16 17	KLALVRIMON SFKLCke KLALVRVI ON SFKPCke KLALVRVI ON SFKPCke KLALVRVI ON SFKPCke	tq-VPLKLGK QG1LQPEKPI V1kvvsrdgi tq- <u>IPLKLRF GG1LLTEKPI V</u> 1kaesrdet tq- <u>IPLKLNA QG1IQPEKPI V1kveprdgs</u> tq- <u>IPLKLTT QG1TQPEKPV V1ki1prdgt</u>	irga vsga vnga vsga	(503)
15 16	KLALVRIMON SFKLCke KLALVRVI ON SFKPCke KLALVRVI ON SFKPCke KLALVRVI ON SFKPCke	tq-VPLKLGK QGllQPEKPI Vlkvvsrdgi tq- <u>IPLKLRF GGllLTEKPI V</u> lkaesrdet tq-IPLKLNA QGlIQPEKPI Vlkveprdgs	irga vsga vnga vsga	(503)

FIGURE 1

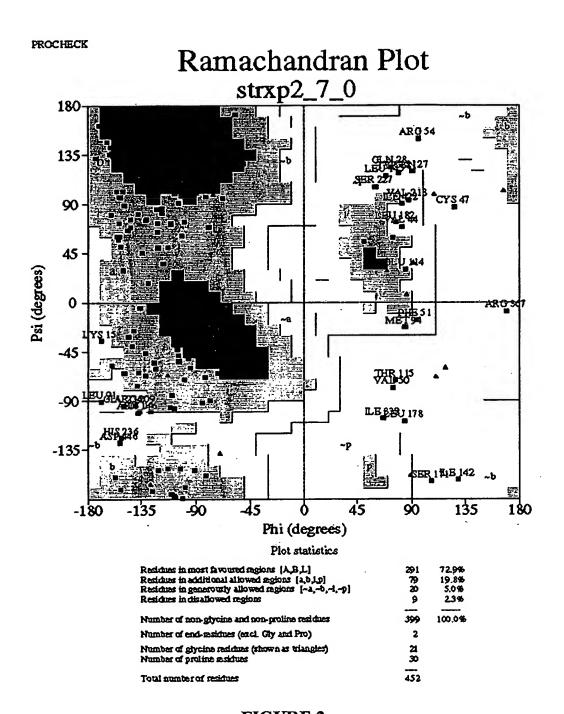


FIGURE 2

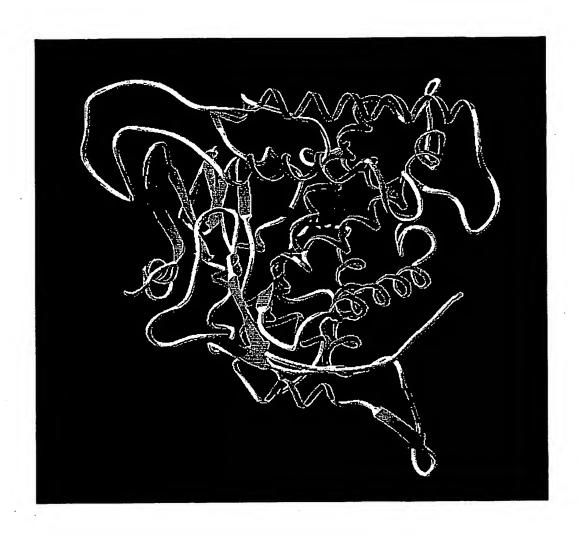
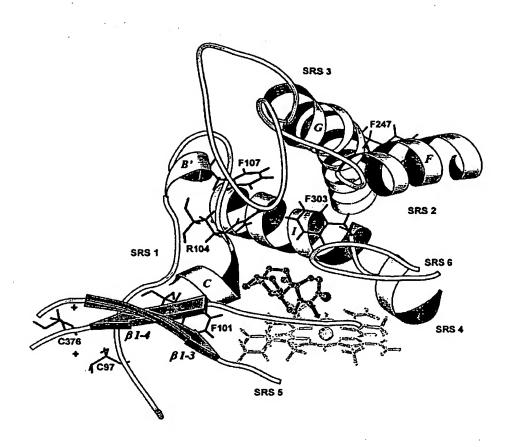
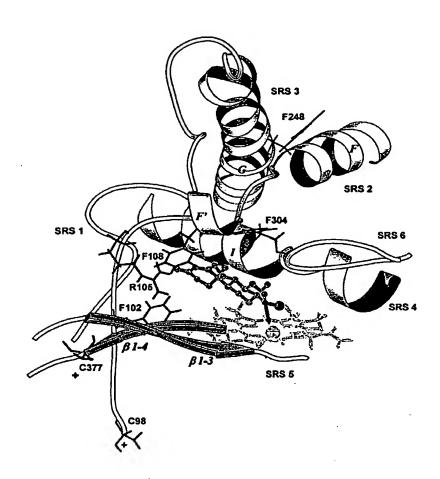


FIGURE 3



Testosterone
16
$$\alpha$$
HO
Testosterone
3A4

FIGURE 4A



Testosterone

OH

16
$$\alpha$$

HO

3A7

FIGURE 4B

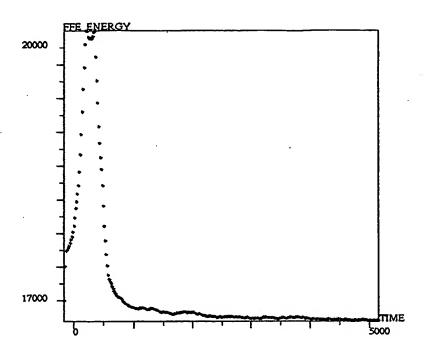


FIGURE 5